Enterprise Systems Analysis

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1 INTRODUCTION

The purpose of the Enterprise Systems Analysis line of research is to develop and evaluate a methodology for modeling and analyzing enterprise systems. We define an enterprise system as a set of interacting organizations that serve a purpose yet have no locus of control. Their behavior is often complex and must be viewed simultaneously from several different perspectives to be understood. The US Department of Defense (DoD) faces a number of challenges where there are multiple interacting organizations with no central locus of control. For example:

• Combating the proliferation of counterfeit parts in military systems
• Managing joint and international acquisition programs
• Coordinating disaster and humanitarian responses involving governments, NGOs, and US agencies
• Sustaining the defense supplier base in the face of declining acquisition quantities

Consequently, DoD has requested research to enable DoD and Government policy makers to better understand these enterprise problems and shape policy appropriately. More specifically, any enterprise systems analysis methodology should enable:

• Representing the "as-is" enterprise, the "to-be" enterprise, and the path between them
• Understanding relationships between variables and techniques for projecting outcomes and performance
• Providing a means for experimentation and creation of response surfaces for analysis of key tradeoffs
• Providing a systematic method to search for policy tipping points and identify counter-intuitive results
• Creating an interactive environment for discussion and debate of strategies, policies and plans
• Enabling key stakeholders to understand the implications and potential second order effects of policy and resource decisions

The work performed during this research task (RT-161) is direct follow-on to the work performed during RT-138 and RT-110. The outcome from the prior work was a shift in emphasis away from building a unitary enterprise model toward a core-peripheral approach in which "peripheral" models could be added or removed as needed to generate scenarios of interest to enterprise stakeholders. Also highlighted, via a series of peer-reviews, was that the methodology needed to be enhanced to better detect unintended or counter-intuitive policy consequences and to better deal with multi-scale ontologies. Consequently, the major tasks for RT-161 were:

1. Apply the core-peripheral approach to a case study of protecting critical infrastructure (Section 3)

2. Develop and validate counter-intuitive results, secondary effects, and policy tipping points (Sections 5 and 7)

3. Extended canonical phenomena and model reuse methods to include multi-scale ontologies (Sections 4, 5, and 6)

4. Update the enterprise analysis methods to incorporate the results of the other tasks (Section 8)

From the execution of these tasks, we were able to develop a fairly substantial update to the enterprise modeling methodology. More specifically, we found from the application of the core-peripheral approach to the critical infrastructure case study that the peer reviewers were interested in using the model for analysis and insight. This is in contrast to the results of the counterfeit parts case study (RT-138, RT-110) where the peer reviewers tended to focus on the use of the model for communication. While this is by no means an absolute validation of the core-peripheral approach, it is an encouraging result. Beyond the case study, a theoretical investigation yielded insights on to how to partition an enterprise system across multi-scale ontologies to generate the core and peripheral models as well as how they should be used together to detect the unintended consequences of a policy. Ultimately, this lead to the revision of the enterprise modeling methodology that reorganized the ten-steps into three major phases. Each phase contains a number of more detailed steps that should provide additional guidance to enterprise analysts. Finally, we also identified a number of promising avenues for future research to better improve the efficacy and applicability of the enterprise modeling approach.

The remainder of this report is organized as follows: Section 2 briefly reviews the findings of RT-138 and RT-110 to explain and motivate the work performed during RT-161. Section 3 presents the results of applying the core-peripheral approach to a case study of critical infrastructure protection. Section 4 summarized the results of an Industry-Government workshop held to discuss the challenge of model centric-engineering approaches which share the same technical and organizational challenges as model-based enterprise analysis approaches. Section 5 provides a detailed literature review of how multi-scale ontologies are modeled and how counter-intuitive results are detected in both the physical and social sciences. With regard to the multi-scale ontology aspects of the problem, Section 6 develops a detailed mathematical analysis of the problem to suggest necessary conditions as well as approaches to mitigate the challenges of modeling across multiple scales. With regard to detecting counter-intuitive results, unintended consequences, and policy tipping points, Section 7 develops a proposed approach to partitioning a multi-scale ontology into core and peripheral models. These models are then systematically varied to generate scenarios that may identify counter-intuitive results. This also led to the identification of a hypothesized approach to organize, navigate, and select models for reuse. However, much additional research is required and promising directions for future research are identified. Based on the results of all of the other tasks, Section 8 presents a revised and enhanced version of the enterprise modeling methodology. Finally, Section 9 concludes the report.

2   IMPLICATIONS FROM PRIOR WORK

The research approach taken in RT-161 was largely driven by the findings of the previous research tasks RT-138 and RT-110 (Pennock et al 2015, Pennock et al 2016). The primary of objective of those studies was to evaluate and refine a ten step modeling methodology for understanding enterprise systems (Rouse 2015). The modeling methodology was evaluating by applying it to a case study of counterfeit electronic part intrusion into a supply chain.

As the counterfeit parts model was presented to different stakeholder groups, the reception was decidedly mixed. Some felt the model would be useful to explore policy options. Others felt that the model told them what they already knew. Many of the comments and observations were familiar to anyone who has been involved with simulation development: concerns about model fidelity, identification of additional phenomena that could be added, concerns about data availability, concerns about predictive accuracy, etc.

It was generally recognized that a model of an enterprise system should not be used to make specific, quantitative predictions. Rather the interest seemed to be in finding counterintuitive results or unexpected consequences. However, the outputs of the simulation were largely what was expected. In some sense, this should not be surprising. Simulations are purely deductive, and thus, the conclusions are necessarily entailed by the premises. This does not mean that one never obtains unexpected results from a simulation, but when one attempts to build a relatively simple and interpretable simulation model that is consistent with the available data and validated via comparison to the predictions of subject matter experts, the likely outcome is a simulation that produces exactly what the subject matter experts said would happen. This is somewhat similar to testing a model against the training set data. Under these circumstances, any unexpected results are purely incidental.

Instead, there seemed to be a sense that the simulation provided a mechanism to both integrate and communicate the inputs of a diverse group of subject matter experts to stakeholders and policy makers. Thus, while the consequences of any given policy option may not be unexpected for some of the subject matter experts, they may be unexpected for a subset of the stakeholders. As a result, the simulation becomes a means to facilitate communication and discussion as well as rule out bad policy options quickly.

Interestingly, the issues encountered during this effort may not necessarily be consequences of the ten-step methodology *per se* but rather the reigning paradigm for simulation development in engineering and the hard sciences. Informally, that paradigm can be described as follows: Build a simulation that faithfully captures the structure of the problem and can reproduce the available data. Such an approach is implicitly designed to maximize predictive accuracy *ceteris paribus*. This is tantamount to trend extrapolation. However, few would argue that simulations of enterprise systems should be used for making specific quantitative predictions. So what are they for? Why is anyone interested in them at all?

Based on our case study, we can see two applications that are not entirely consistent. First, the simulation can serve as a means to integrate and communicate data and expertise from diverse sources. In this case, the knowledge to "extrapolate the trend" exists, but it is scattered. This knowledge is captured, encoded, and integrated via the simulation development effort. Once this is accomplished, stakeholders and decision makers can explore this encoded knowledge in a way that is not possible via multiple separate conversations with subject matter experts. Unexpected or counterintuitive results may pop out, but these will be by-products and chances are they will be counterintuitive to some but not all. Thus, the simulation serves more as a thinking aid for group decision making as opposed to a means to discover something truly surprising.

The second application is to identify counterintuitive results and unintended consequences of policy options. Since we are fairly effective at trend extrapolation, the goal shifts from reproducing the trend to trying to identify what might cause the trend to change. How could our well intentioned, well thought out policy go wrong? This is exactly the opposite of fitting a model to data or subject matter expert predictions. Instead we want to understand the feasibility of scenarios that we have not experienced or run against conventional wisdom. In other words, we are not just interested in the data. This suggests a very different way to go about building a model.

If the objective is really to identify counterintuitive results and unintended consequences, then the reigning paradigm for developing simulations in engineering and the hard sciences may be suboptimal for this purpose. Instead, we could take a page from the field of risk analysis. We want to consider how we could make a policy produce unexpected outcomes. This entails deliberately exploring variations of conventional assumptions, experimenting with alternative referential ontologies and theories, and hunting for feedback effects. As noted by Cardoso and Pennock (2016), this is analogous to efforts to use system dynamics to identify unintended consequences in policy analysis. The difference is that here we would vary more than just balancing and reinforcing loops as we are intentionally considering various ontologies and scales.

From an epistemological standpoint, we have no guarantee that any unexpected results identified can or will happen. Instead they simply establish the possibility. Once these are identified, they can be adjudicated and investigated further. To put it succinctly, rather than trying to build a model that faithfully reproduces what we see, it should be giving us guidance as to where to look.

One could argue that enterprise modeling methodology evaluated in the two preceding SERC tasks is a product of the reigning paradigm. Consequently, it is more suitable for the first application than the second. This may explain, in part, why the counterfeit parts simulation generated more interest as a communication tool than a means to find unexpected policy consequences. However, the methodology seems to be flexible enough to accommodate the second application as well.

To accommodate the idea of using the simulation to identify unintended consequences, we modified the modeling approach based on the lessons learned from the counterfeit parts case study. This modified approach was then evaluated in this research task via a case study of critical infrastructure protection. We found in RT-138 that the using a multi-level view of the enterprise is useful for conceptualizing the enterprise, but we suspect that the output metrics of interest are usually the direct output of one or two of the layers. Thus, it makes sense to create an integrated core model that generates the values of these output metrics. We could consider the core model the first order logic that governs the values of the output metrics.

We are then interested in searching for higher order effects that one might consider counterintuitive results or unintended effects. The natural place to find these are via interactions with the other layers. However, there may be more than one way to represent the other layers. This is particularly true for human and social behaviors. Returning to the counterfeiting example, should we model counterfeiters as classical utility maximizers? Should we employ prospect theory? Information economics? Each approach may reveal a different insight. More importantly, each may have a different impact on the behavior of the core model.

Thus, we represent the non-core layers using peripheral models. The purpose of the peripheral models is to "perturb" the core model to generate useful insights. A major risk to implementing a policy option in an enterprise is crossing a tipping point that no one knew was there. The peripheral models can be used to trigger tipping points in the behavior of the core model. Finding the tipping points depends on exploring structural and ontological variations of the peripheral models (Pennock & Gaffney 2016).

While the natural tendency in enterprise modeling seems to be to maximize predictive accuracy by maximizing the fidelity of the model (i.e., add as many relevant factors as possible), this approach has rapidly diminishing returns as it increases the degrees of freedom and risks over-fit with sparse data (Pennock & Gaffney 2016). Rather, it may be more productive to build a relatively simple core model and then selectively perturb it with structural variations in the peripheral models to see if this triggers any unexpected behaviors (e.g., tipping points).

Evaluating and refining this core-peripheral approach to detect unintended consequences of a policy is the primary objective of this research task. The remainder of this report documents those efforts. The key elements were:

- A case study of protecting critical infrastructure to evaluate the mechanics of the core-peripheral approach (Section 3)

- An industry-government workshop to understand the state of practice in model centric engineering (which is an analogous problem to using multi-level model to find unintended consequences), (Section 4)

- A detailed literature review of how multi-level issues are handled in the physical and social sciences as well as how unintended consequences and counterintuitive results are detected (Section 5)

- A set-theory based analysis of the mathematics behind developing a valid multi-level model (Section 6)

- Initial development of an approach to systematically identify unintended consequences (Section 7)

Ultimately, the results of these efforts led us to propose changes to the ten-step enterprise modeling methodology (Section 8).

3 CRITICAL INFRASTRUCTURE PROTECTION CASE STUDY

Case studies have been used in this research as a primary method to aid in evaluation of enterprise modeling methodologies. Here, we discuss a case study model involving critical infrastructure.

3.1 BACKGROUND

Critical infrastructure includes such systems as the power grid, communications networks, transportation networks, food delivery systems, financial systems, emergency response systems, and numerous others. These systems, as the name implies, have become essential to the operation of modern society, as well as to national defense. At the same time, critical infrastructure systems have become extensively interconnected and networked. While there are clear benefits to the functionality of infrastructure from this interconnection, the interdependencies introduced can create vulnerabilities that are difficult to identify and safeguard. These vulnerabilities may be due to unintentional failures (e.g., faulty or aging components) or to intentional actions (e.g., terrorism, cyber-warfare, etc.). Once a failure occurs, it can cause cascading failures in other systems and infrastructures due to interconnections.

With the increased importance of infrastructure, plus a number of high-impact failures in recent years, a significant body of research has studied the design, behavior, performance and vulnerabilities of these systems. This research has largely focused on the technical aspects of these factors. Like many complex systems-of-systems, though, critical infrastructure operates in an enterprise context. That is, critical infrastructure is not a monolithic system, but different parts of these infrastructure systems are owned and operated by different firms or agencies. In addition, regulatory agencies and other organizations interact to influence behavior of different actors. This collection of organizations is an extended enterprise concerned with safe and effective operation of the interconnected infrastructure systems.

Critical infrastructure was established as a national priority in the 1990s with a number of directives, including Presidential Decision Directive NSC/63 (White House, 1998). This directive established a public-private partnership for managing and protecting critical infrastructure, effectively an enterprise consisting of government agencies and private firms. This public-private partnership is detailed in such documents as the National Infrastructure Protection Plan (DHS, 2013).

Here, we explore the behavior and performance of critical infrastructure from an enterprise perspective. In particular, we are interested in the resilience of such systems. We use an enterprise modeling methodology that addresses the socio-technical behavior of the enterprise to create a simulation of the enterprise and use this simulation to study the effects of various policies and external effects.

3.2 MODELING OF CRITICAL INFRASTRUCTURE

The importance and complexity of the problem has inspired a variety of research efforts. For instance, Dehghani and Sherali (2016) develop an optimization approach for scheduling maintenance to mitigate disaster impacts, while accounting for stochastic system behavior. Due to the high level of stochastic behavior, though, most research has focused on simulation. Additionally, systems-of-systems modeling frameworks have been introduced as a way to represent interactions.

Otto et al. (2016) specify a system-of-systems framework for modeling infrastructure to support long-term simulation of these systems. Min et al. (2007) combine IDEF models, system dynamics and non-linear optimization to provide capability to set control variables to minimize the effect of disruptions. Grogan and de Weck (2015) propose a systems-of-systems modeling framework to support simulation of infrastructure systems.

Several in-depth reviews of modeling methodologies and applications for critical infrastructure have been published (Ouyang, 2014; Pederson et al., 2006; Yusta et al., 2011). These reviews highlight the role of agent-based simulation in addressing individual decision-makers and the bottom-up nature of many infrastructure-related phenomena, plus the role of system dynamics simulation in addressing non-linear phenomena and feedback loops. In particular, agent-based approaches are well-suited to modeling enterprise systems, since complex agents can represent the different enterprise actors (firms, agencies, etc.). Most approaches that use agent-based modeling, however, use agents for individual decision-makers and system elements. One exception involves a large-scale architecture for composing models of different infrastructure systems for different analyses with a focus on socio-technical behavior (Atkins et al., 2008). Fujimoto et al. (2016) discuss perspectives on applying dynamic data driven application systems to simulation of smart cities and infrastructure grids whereby system data drives simulation (DDDAS) computations that provide dynamic adaptation to improve performance.

Pederson et al. (2006) distinguish between single models versus coupled models. Single models combine different infrastructure systems into one model, while coupled models feature a coupled collection of models, each with a single infrastructure. Additionally, some models couple with earthquake models or other disaster models or with database information such as GIS. Large-scale models often suffer from long run times. Rosen et al. (2016) report on an approach using neural network metamodels and stochastic krieging metamodels to improve model response times for decision support in critical infrastructure network evaluation.

Many of the studies above use system availability or recovery from disruption as measures of infrastructure performance. Increasingly, though, research has focused on resilience as a

performance measure for infrastructure systems, with definitions metrics. Hosseini et al. (2016) review various resilience definitions and metrics and distinguish between qualitative frameworks and quantitative approaches. Francis and Bekera (2014) propose a metric based on three types of resilience – absorptive, adaptive and restorative. Absorptive resilience refers to the ability of a system to absorb a shock and not lose performance significantly. Adaptive resilience refers to the ability of a system to reconfigure itself to minimize the impact of a shock. Finally, restorative resilience refers to the ability of a system to return to an acceptable or nominal state of performance quickly after a shock.

Similar to the counterfeit parts case study, there are a number of features that make this an enterprise problem.

- There is no locus of control.
  - Each sector of critical infrastructure is overseen and regulated by a different federal agency. For instance, the Department of Energy addresses the power grid. Department of Homeland Security oversees the communications infrastructure.
  - Private firms manage different parts of the various infrastructure networks.
  - These firms typically operate at the state level rather than the national level and are regulated by state agencies.
- There is significant adaptive behavior.
  - Terrorists may adapt to different strategies to protect infrastructure.
  - Populations adapt to infrastructure outages and potential outages.
- There is significant complexity.
  - Clearly, there is significant socio-technical behavior from the market. Socio-technical behavior is inherently complex.
  - In addition, there are multiple interconnected infrastructure systems that interact, with sometimes unpredictable effects.

3.3 METHODOLOGY

In recent years, there has been growing interest in modeling and analyzing enterprise systems. An enterprise is a collection of organizations and resources that cooperate in pursuit of some goal or mission (Rouse, 2005). To address improved enterprise performance, a variety of research efforts have created methods to model and analyze enterprise systems (Barjis, 2011; Gharajedaghi, 2011; Giachetti, 2010; Glazner, 2011), with a focus on design or transformation of the enterprise.

Our primary interest has been on generic and reusable methods for modeling enterprises. One approach to modeling the variety of enterprise phenomena is to consider different levels of enterprise organization and behavior. Enterprises are often conceptualized as operating at a macro-level, with different agencies, firms and other organizations interacting to support a common goal in the context of a larger economy. However, they also operate at a micro-level with the transactional delivery of products and services to individual consumers. In between these two levels, enterprises can be decomposed into a number of elements and activities,

including units within organizations, supply chains supporting the transformation of raw materials to delivered products and services, and workforces that perform the activities supporting enterprise goals. Thus, enterprises can be represented as multi-level systems.

Such a multi-level formalism and associated modeling methodology are proposed by Rouse (2015). The formalism features an eco-system level, a networked inter-organizational structure level, an operational delivery level, and a work practices level. The methodology then has ten steps, starting with abstract modeling, then moving to composition of multiple modeling formalisms needed for various enterprise phenomena, and finally addressing traditional issues of parameter estimation, model building, and verification and validation.

A modified version of this methodology was proposed by Pennock et al. (2017) based on results of our previous case study addressing counterfeits parts in the DoD supply chain. The next sub-sections describe the application of this revised methodology to critical infrastructure via a series of steps. The focus is on the first series of steps in modeling as opposed to the later stages of data gathering, model implementation, and experimentation.

3.3.1 CENTRAL QUESTIONS OF INTEREST

The first step of the methodology is to decide on the central question(s) of interest. This question relates to the intended use of the model. In an enterprise problem context, this step also incorporates the perspectives of multiple stakeholders and potentially multiple uses. Thus, it may not be as obvious as for a model of a purely technical system with one or two stakeholders

The model is intended to address the following question: what is the best mix(es) of investments, standards and policies for providing long-term value in terms of availability, safety and security versus cost.

3.3.2 KEY PHENOMENA

The next step in the methodology is to characterize the key phenomena that should be represented. Based on the literature review discussed previously, key phenomena are organized into several different categories as shown below in Table 1.

Table 1. Key phenomena for critical infrastructure

Category	Phenomena of Interest
Infrastructure systems	• Infrastructure nodes • Network architecture linking node • Service delivery between nodes • Redundancy, hardness • System performance criteria • Maintenance and repair schedules

Infrastructure system inter-connections	• Relationships and dependencies from one infrastructure system to another
	• Effects of outages in one infrastructure system to another
Enterprise actors	• Firms that own segments of infrastructure
Policy	• Federal agencies
	• State regulations
	• Redundancy/hardness
	• Foreign ownership
Exogenous factors	• Technological progress
	• Threat profiles

Table 1 focuses on generic elements for infrastructure systems. The model implemented here addresses the electrical grid, water delivery systems, and the internet communications grid. The elements above are therefore specialized for purposes of representing these infrastructure systems. For instance, the service provision of the electrical grid is power, and the service provision of the water delivery system is drinkable water. The internet provides communications via data packets. The electrical grid consists of power plants, transmission lines, substations, distribution lines, and demands. The water delivery system consists of sources, reservoirs, treatment plants, pipes, and demands. The internet system consists of servers and network cabling.

3.3.3 VISUALIZATIONS OF RELATIONSHIPS AMONG PHENOMENA

The multi-level modeling construct has been useful in conceptualizing different phenomena and how they operate at different levels. The four levels consist of the eco-system, the system structure, delivery operations, and work practices. In this effort, the focus is largely on the system structure and delivery operations. Work practices come into play implicitly when repair and maintenance is conducted or when services are delivered, but these are not modeled in detail. The eco-system influences the behavior and performance of the infrastructure systems, often in an exogenous manner. Figure 1 shows a visualization of the multi-level model for critical infrastructure.
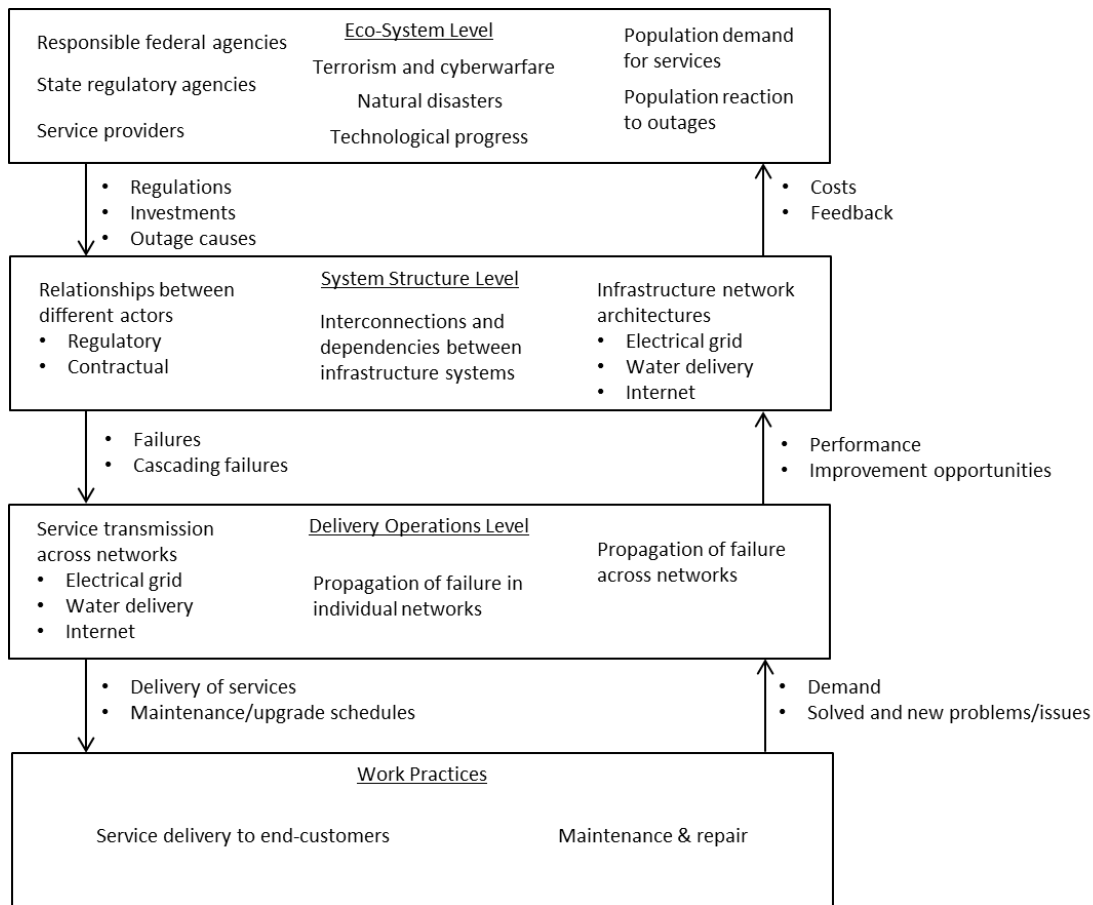
Figure 1. Conceptual enterprise model of critical infrastructure

3.3.4   KEY TRADE-OFFS THAT APPEAR TO WARRANT DEEPER EXPLORATION

Next, key trade-offs are articulated so that the phenomena underlying them can be included. The following trade-offs were identified for critical infrastructure.

- Trade-off between resilience and cost for different levels of redundancy and protection via hardness;

- Trade-off between resilience and cost for different strategies of upgrading technologies and standards;

- Trade-off between service level and resilience for different architectures and interconnection patterns.

3.3.5   ALTERNATIVE REPRESENTATIONS OF THESE PHENOMENA

Simulation modeling provides three primary paradigms – discrete-event (DE), agent-based (AB) and system dynamics (SD). Discrete-event models focus on events, processes that cause events, and new events triggered by executing events. Agent-based models focus on elements within a model, how they react to messages and state changes, and how system behavior

emerges over time as a result of individual element behaviors. System dynamics models address rates of change, interdependencies, feedback loops and lags in system behavior. Table 2 shows alternative modeling representations for the categories of enterprise elements in Table 1.

Table 2. Alternative modeling representations

Category	Representation alternatives
Infrastructure systems	- Agent-based – AB models provide support for state transitions to model the node state behavior and inheritance to model different types of nodes with commonalities, plus message-passing between nodes. - Discrete-event – DE models provide support for discrete elements moving through processes representing infrastructure networks. There is limited support for inheritance and message-passing (except through signal-hold). - System dynamics – SD models provide support for continuous flows found in many infrastructure systems. - Agent-based and system dynamics models are preferred due to their complementary support for state-based behavior and continuous flow.
Infrastructure system inter-connections	- Agent-based – AB models support message-passing between different infrastructure systems. - Discrete-event – DE models support discrete elements transitioning between infrastructure systems and signal-hold for message-passing. - System dynamics – SD models support continuous flow between infrastructure systems. - Agent-based models are preferred due to the flexibility of their message-passing capability over discrete-event models, and due to the discrete nature of on-off relationships that exist for service provision between infrastructure systems.
Enterprise actors	- Agent-based – AB models have been used extensively to model interactions of individual units, as well as adaptive behavior. In addition, there is potential to embed micro-economic models in agents. - Discrete-event – DE models are not typically used for enterprise actor models. - System dynamics – SD models are not typically used for enterprise actor models. - Agent-based models are preferred due to their extensive use in modeling individual unit interactions, adaptive behavior and economic behavior.

Policy	• Agent-based – AB models have been used extensively to model interactions of individual units, as well as adaptive behavior. This could extend to policy units. • Discrete-event – DE models are not widely used for policy models as are AB and SD models. • System dynamics – SD models have seen extensive use for policy study, with the concept of variables being used as policy levers having resulting interaction effects. • Agent-based models are preferred do to the ability to represent adaptive behavior of policy-makers. Policies would be represented as variables, with the policy effects embedded in other sub-models.
Exogenous environment	• Agent-based – AB models support exogenous elements such as organizations/actors. • Discrete-event – DE models support exogenous elements involving process behavior. • System dynamics – SD models can be used to aggregate behaviors and incorporate feedback loops, lags, etc. SD models have been used for macro-economic phenomena. • Agent-based and system dynamics models are preferred due to, respectively, their representation of organizations/actors, and their representation of aggregate effects not requiring detail.

Table 3 presents descriptions of the representations selected for different categories of phenomena being modeled.

Table 3. Selected representations

Category	Phenomena of Interest
Infrastructure systems	Agent-based model for nodes and arcs. System dynamics models and similar continuous flow models embedded into agents for service flow.
Infrastructure system inter-connections	Agent-based network of connections with message-passing for state-change notifications.
Enterprise actors	Agent-based model with actors modeled as complex agents and relationships modeled by message-passing.
Policy	Global variables set by analyst with associated agent-based policy actors to enable policy adaptation.
Exogenous environment	Agent-based and system dynamics models representing trends in technology progress, technology off-shoring.

3.3.6 ABILITY TO CONNECT ALTERNATIVE REPRESENTATIONS

The representations in Table 3 consist of agent-based and system dynamics representations. These two paradigms can interoperate via such simulation platforms as AnyLogic™, where both formalisms are supported in underlying Java™.

The key is to design the interaction so that it is computationally efficient and scalable. For instance, such interactions can occur via condition-checking or by message-passing. With condition checking, a variable is monitored continually, and when it reaches a threshold, an event is triggered. This can be computationally intensive if there are numerous such variables being monitored. Thus, message-passing is typically preferred.

3.3.7 CORE MODELS AND PERIPHERAL MODELS

Our approach uses a "core-peripheral" method to construct the overall model, similar to the approach used in the counterfeit parts enterprise model. The core model consists of the set of phenomena that are central to the enterprise. Peripheral models are developed to support specific analyses of interest. For instance, in the counterfeit parts model, the core model consists of the defense supply chain, the systems and constituent elements supported by the supply chain through manufacturing and sustainment, and the enterprise actors that own and manage different parts of the supply chain. One peripheral model addresses the recycling of electronic waste. Often, this waste is exported to third-world nations, and some of it is processed into fraudulent counterfeit electronics that are imported into the U.S. The peripheral model addresses the behavior of the recycling market when export restrictions are put in place.

Here, the core model consists of the different infrastructure systems and their inter-connections, plus the set of enterprise actors and policy actors that interact with the infrastructure systems. This core model can be considered as the "steady-state" representation of the infrastructure systems. The peripheral models, on the other hand, represent disruptive factors such as terrorism or a natural disaster. It is the effect of these peripheral models on the core model that is of interest (as well as what protections and recovery mechanisms are represented in the core model). This is somewhat different than the approach taken in the counterfeit parts model, since the disruptive forces (i.e., counterfeiters) are part of the core model, being part of the supply chain.

Figure 2 shows the model architecture with the core model and various peripheral models.
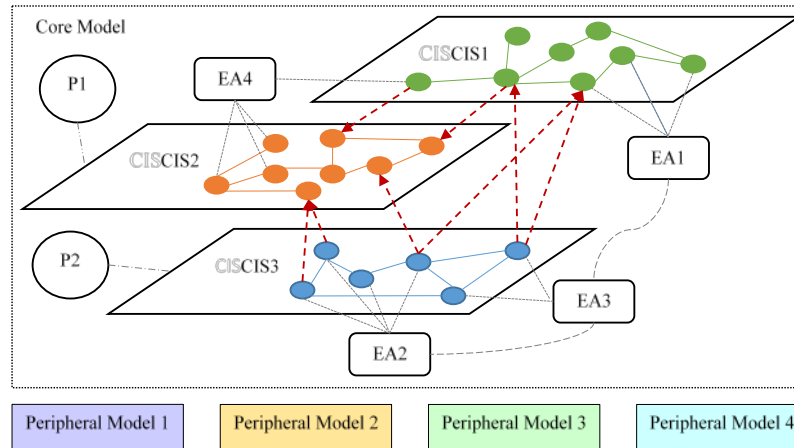
Figure 2. Model architecture

The next section provides details on the model implementation.

3.4 MODEL DESCRIPTION

A prototype enterprise simulation for critical infrastructure has been implemented using AnyLogic® 7. AnyLogic is a commercial simulation software package that provides capability for multi-method modeling of complex systems using agent-based, discrete-event and system dynamics. As such, it is useful for enterprise modeling.

3.4.1 INFRASTRUCTURE SYSTEMS

Three different infrastructure systems are modeled – the electrical grid, the water delivery system, and the internet portion of the communications system.

The electrical grid sub-model starts with a set of power plants. These can be based on coal, gas, oil/gas, or nuclear power. They provide power to a set of transmission sub-stations via high-voltage transmission lines. High-voltage enables less current and power loss due to resistance over the long distances of power transmission. These sub-stations are nodes in the transmission network. Sub-stations can transmit power to other transmission sub-stations, depending on the layout of the transmission network. Eventually, a transmission sub-station will link via a transmission line to a distribution sub-station. Distribution sub-stations reduce the voltage of the power transmission via transformers so that it can be supplied to customers. A set of distribution lines then distributes power to industrial and residential demand sources.

The power plants are implemented as agents having a set of outbound transmission lines and a certain megawatt rating. In addition, they have state-based behavior as shown in Figure 3.
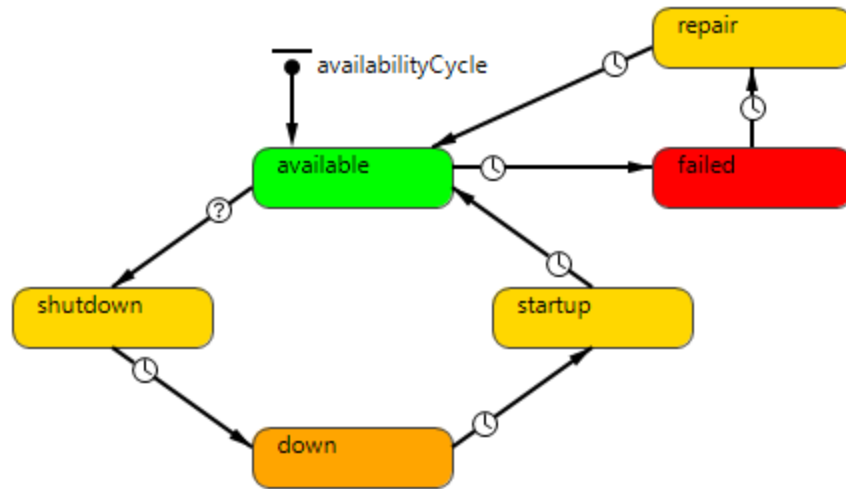
Figure 3. Power plant availability cycle

The transmission and distribution lines are also implemented as agents. These agents have simple system dynamics models embedded to represent the continuous flow of current and power through the line. There are two variants of transmission and distribution lines. In the simplified version, the concern is whether power is supplied or not to the line. The second is more detailed, and it contains a direct current representation of power flowing through the distribution network. This is an approximation for the alternating current power grid. In this variant, electrical concepts modeled include voltages, resistance and power loss. This is depicted in Figure 4.
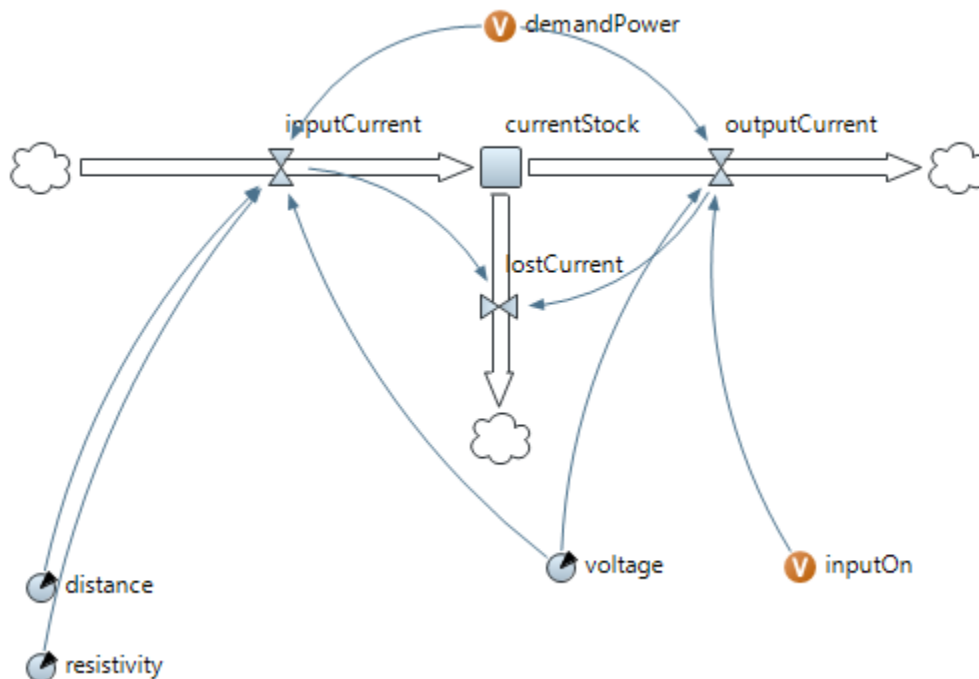
Figure 4. Power line using DC transmission model

A demand source has a number of businesses or residences that it serves, plus a state-based demand model that changes the level of demand during the day. If an upstream system element fails, power is turned off to downstream elements. Once the failure is resolved, the downstream elements receive power again.

The water delivery system starts with water sources and reservoirs. Pipes connect these sources and reservoirs to treatment plants. Once water is treated, it is supplied to water tanks via pipes. These tanks then supply water to industrial and residential customers. The water delivery system is modeled using the AnyLogic fluid library. This library offers continuous flow constructs similar to stocks and flows in systems dynamics. Similar to the electrical grid sub-model, these fluid elements are embedded into agent objects to provide state-based behaviors, plus encapsulated variables.

Water sources are modeled using fluid sources embedded into water source agents. Reservoirs and water tanks are modeled using tanks that are embedded into reservoir and water tank agents. Tanks are temporary storage elements in the fluid library. Pipes are modeled using pipeline elements encapsulated in pipe agents. Demand sources are modeled as agents with embedded fluid-dispose elements. The demand sources have a demand variable, plus a variable to denote either the number of residences or businesses served.

The two agents that can fail in the water delivery system sub-model are treatment plants and pipes. We assume that water sources, reservoirs, and tanks do not fail. If a water treatment plant or a pipe fails, downstream elements will receive fluid temporarily, but then will eventually run out until water service is restored by a fix to the failed element.

In addition to failures, water can be contaminated. If this occurs, it is assumed that a particular reservoir or tank is contaminated. The tank or reservoir is unavailable until a remediation process fixes the contamination problem.

The final infrastructure system is the internet. The internet operates in a tiered fashion with major telecommunications companies operating at the top level (Tier 1) with data exchange between their networks. Tier 2 internet service providers link directly to this network and provide service to their customers. A Tier 2 network operates between the Tier 1 network and the smaller Tier 3 ISPs. A Tier 3 ISP may be single-sourced or multi-sourced in terms of its connections to the Tier 2 network elements. A large company or organization is considered a Tier 3 ISP in that it connects to a Tier 2 network element and provides its own internal networks and services.

Tier 1 telecommunications providers and Tier 2/3 ISPs are modeled as agents. These operate as nodes in the internet network. They have server agents that provide processing capacity for transmission of packets that comprise internet traffic. They are connected via arc agents that model packet transmission. Servers and arcs have state behavior, and they are either in an "available" state or in a "failed" state.

The various infrastructure networks are populated via a relational database that contains the node-link relationships. This database is read by the simulation model at start-up to initialize the infrastructure systems.

3.4.2   INFRASTRUCTURE SYSTEM INTERCONNECTIONS

These three infrastructures have several different types of interconnections and dependencies as summarized below.

- The electrical grid supplies power to water treatment plants. Such plants are industrial customers.

- The electrical grid supplies power to servers in various parts of the internet architecture.

- The internet supplies real-time information to the electrical system. Without such real-time information, response times may take longer.

- The internet supplies real-time information to the electrical system. Without such real-time information, response times may take longer.

3.4.3   ENTERPRISE ACTORS

The enterprise actors consist of the various actors in the infrastructure system infrastructure that provide services. They are modeled as decision-making agents. There are four types of enterprise actors in the current model:

- Power providers

- Water providers

- Telecommunications firms

- ISPs

The enterprise actors implement policy directives for their segments of infrastructure systems. This implementation takes time, and it is influenced by the provision of subsidies and restrictions on foreign ownership of firms that may perform upgrades to meet directives.

3.4.4   POLICY

Policy actors consist of those federal agencies that oversee the different infrastructure systems. These are modeled as complex agents that issue policy directives. Policies currently modeled include the following:

- Restrictions on foreign ownership of infrastructure-related firms (including contractor firms that perform upgrades, etc.).

- Redundancy requirements for certain infrastructure elements

- Hardness requirements for certain infrastructure elements

- Subsidies for infrastructure hardness or redundancy

At present, state regulatory agencies are not modeled. However, they could be added in the future if regulation is of interest.

3.4.5 PERIPHERAL MODELS

Currently, two peripheral models are implemented.

- Terrorism – In this sub-model, segments of infrastructure systems are targeted for outages. The success of these outages depends on the hardness and redundancy of the segment targeted. Terrorists have limited knowledge of hardened or redundant assets, and thus they seek to target assets that have limited hardness or redundancy.

- Natural disaster – In this sub-model, a natural disaster is represented as a failure in multiple infrastructure systems within a geographic area. This could be due to an earthquake or a flood, for example.

3.4.6 PERFORMANCE

The model tracks two primary performance measures.

- Resilience: Resilience is the ability of an infrastructure system to avoid reductions in service delivery or recover from service delivery problems due to a disruption. Currently, resilience is measured as simply the system availability relative to its capacity over time. As the model is matured, other more sophisticated measures will be introduced such as the metric in Francis and Bekera (2014).

- Cost: Accrued cost over time is tracked to determine the expense associated with different policies. Cost can be considered as multi-dimensional similar to service level.

3.4.7 USING COUPLED MODELS

The core model has been developed as an integrated model of different infrastructure systems. In scaling up this modeling approach, it may be necessary to compose different existing models of different infrastructure systems. Pederson et al (2006) discusses examples of such model compositions. In this section, we briefly discuss model composition issues from the perspective of the current model, assuming that different infrastructure systems are modeled separately.

In this model, the interactions between different infrastructure systems are based on services provided from one infrastructure system to another. For instance, the electrical grid model provides power service to the water delivery system model, namely to water treatment plants. A state change in the electrical grid model may result in a power outage. This power outage

may cause power loss to a water treatment plant. In the integrated model, the water treatment plant is a power demand source in addition to being a water treatment plant. The segment of the electrical grind that experiences a failure sends an outage message that is propagated to downstream elements of the grid. The power demands receive this message and can adjust their state to power-off. Similarly, when power is restored, a message is sent to downstream elements notifying

Assuming two composed models (electrical grid and water delivery system), the state of the electrical grid model is input into the water system model. The linkage between the two models is therefore a state-linked relationship (See Section 6). Since outages are not a continuous occurrence, the computational burden associated with managing the state-linked relationships between this pair of composed infrastructure models is likely manageable. As the number of infrastructure models included increases, this would scale with the number of pairs with dependencies (n), the number of dependencies in each system pair (m), and the average frequency of state-change (f) to be $O(nmf)$. Dependencies are assumed to be one-way here.

Note that the current model has a discrete linkage relationship. If the input-output relationships are based on the values of continuously changing variables, the computational burden would increase due to increased f.

The power demands not associated with other infrastructure systems are modeled in aggregate. That is, collections of residences or businesses are aggregated into one demand node. This is also true of water delivery system demands. Thus, for demands at different times, we would use data from each individual infrastructure system to model, for instance, demand in the morning versus demand at night. If we increase the granularity of the model, though, so that a demand represents an individual residence or business, it is no longer the case that independent datasets can be used. For example, one particular residence may not follow the aggregate demand functions due to telecommuting. Thus, water usage and electricity demand would depend on one another, and the power demand node in the electrical grid model would be linked to the corresponding water demand node in the water delivery system. To account for the individualized behavior of a residence or business, the existing composition would have transition-linked relationships. Since these linkages are known, they are explicit transition-linkages.

To remediate them, constraints may be put in place. For example, a variable set can be added to one of the demand nodes indicating the type of at-home behavior of that node. This variable set then influences state changes in the demand for its node directly, and it can be used in a state-linked transition to influence the demand in the corresponding node in the other infrastructure model.

3.5 EVALUATION

The model and enterprise modeling approach were presented to a group of subject matter experts involved in the INCOSE Critical Infrastructure Protection and Recovery (CIPR) Working Group. An initial overview was presented to the CIPR-WG at the 2017 INCOSE International Workshop. A second presentation was made to the CIPR-WG's monthly meeting on February 16.

Comments and discussion from this second session were captured and are organized along the following lines:

1. Validity — the extent to which the simulation is technically correct relative to the purposes for which it was developed.

2. Acceptability — the extent to which the simulation addresses problems in ways that are compatible with current preferred ways of decision-making and/or potentially useful new ways of multi-stakeholder decision-making.

3. Viability — the extent to which use of the simulation for the purposes intended would be worth the time and effort required.

Validity

- What data sources are being used? Most data for the various infrastructure sectors is sensitive or proprietary.
    - The data is synthetic in the model currently due to this issue.
    - It would be desirable to have synthetic datasets that were validated as being "representative" of actual datasets for purposes of public analysis.

- Can this approach be used to model micro-grids? There are some opportunities to model these types of systems, which would be on a smaller scale and may provide some validation.
    - This approach should work for micro-grids.

- It would be helpful to see a detailed walk-through of the model, the various parameters, and the interactions.

- This could connect to work being done in model-based systems engineering (MBSE) and in patterns.

- Resilience has many different definitions. The usage of absorptive, adaptive and restorative is interesting.

- It would be of interest to incorporate major disruptive events such as solar flares or electromagnetic pulse bombs into the types of phenomena modeled.

Acceptability

- There was general agreement that this type of modeling approach would be useful for addressing some of the issues that the CIPR-WG community has tasked.

- It would be useful to extend the model to additional infrastructure sectors.

- We need to build up a modeling community for critical infrastructure.

Viability

- Several individuals expressed interested for this as a focus area within CIPR-WG. This could be foundational to creating a community that could sustain this type of modeling.

- What level of effort is involved in creating a model with many different interacting infrastructures?

Overall, the discussion and feedback focused less on using such a model to engage different infrastructure communities from different perspectives to provide a platform for communication and perspective-sharing and more on the use of such models for analysis and insight. This is in contrast to the subject matter expert review of the counterfeit parts case study. Most likely, this is a function of the INCOSE working group in question, in that it focuses on across-domain work in critical infrastructure and thus does not require as much in terms of communication tools for different perspectives.

4   SUMMARY OF INDUSTRY-GOVERNMENT FORUM ON MODEL CENTRIC ENGINEERING

Real world experience is a critical component of developing methods and approaches that can be transitioned to practice. With regard to this effort, relevant real world experience would need to involve both multi-level/multi-scale modeling as well as detection of unintended consequences that result from the interactions of these multiple views of the system. One area where practitioners are addressing these challenges is Model Centric Engineering (MCE). The goal of MCE is to use computer modeling and simulation to capture and manage every aspect of the engineering process from requirements development to design to sustainment. The goal is to use simulation to detect potential issues much earlier in the system lifecycle to avoid costly fixes and workarounds downstream. Necessarily this means computationally representing the system from multiple perspectives and tracing the consequences of decisions in one perspective to consequences in the others. From a technical standpoint, the problem is very similar to that of detecting unintended policy consequences in an enterprise system. The chief distinction is that behavioral social factors tend to play a larger role in enterprise systems than engineered systems. As we will see in Section 5.2, dealing with behavioral and social factors in a multi-level model is a substantial challenge.

To gain an understanding of the state of practice in MCE an industry-government workshop was held in Washington, DC on May 26, 2016. Participants in the workshop included:

- 15 faculty members from across the collaborating SERC universities

- 35 technical leaders from Industry

- 25 technical leaders from the government

The detailed results of this workshop were provided in a separate report to the Government. Consequently, the results will only be summarized here.

While there was certainly discussion of the technical issues associated with developing and integrating the computational models to support MCE, interestingly, much of the discussion revolved around behavioral, cultural, social, and organizational impediments to implementation. In short, while not stated this way by the participants, they felt implementing MCE is largely an enterprise problem. Existing business practices and cultural norms make it nearly impossible to implement MCE even if the technical challenges are overcome. So while the technical challenges were recognized, at least the from the researchers' perspective, they were largely neglected in the MCE forum. Rather, there seemed to be an acknowledgement that how one integrates and validates a multi-level simulation to support MCE is an open research question. There currently exists no systematic approach to accomplishing this. Existing efforts have largely been implemented on a case-by-case basis.

So while the workshop produced limited technical insights on how to accomplish the detection of unintended consequences computationally, it certainly validated the research question. In fact, it revealed that the implementation of MCE itself is an enterprise problem that requires analysis. However, without techniques from practitioners to consider, the importance of understanding the work of those using multi-level or multi-scale models in the physical and social sciences became critical to the research effort. The results of that investigation are presented in the following section.

5   LITERATURE REVIEW

In order to develop of a systematic approach to detecting unintended policy consequences in an enterprise system using the proposed core-peripheral approach, several issues must be addressed. First, the peripheral models are often going to be described using an ontology that is nominally incompatible with the core model because it uses a different abstraction or different scale. Thus, one is concerned with how to handle multi-scale ontologies. Second, enterprise systems contain substantial behavioral and social components. It is likely that one or more of the peripheral models will draw from the social sciences. Historically, models in the social sciences exhibit both greater variance and more instability than those from the physical sciences. Understanding how these issues are handled in the social sciences is critical. Third, building a model from multiple abstractions creates validation issues as the model is built is different from the component theories that have been validated. That validation does not automatically pass to the new composite model. Thus, there is the question of how one knows whether or not the predicted consequences of a composite model are valid. An examination of

how this is handled in both the physical sciences and social sciences is necessary to develop an approach to validate enterprise models.

It should be noted that the social sciences and the physical sciences follow drastically different approaches to modeling systems and predicting outcomes. The social sciences tend to be more data driven to find unintended consequences, while the physical sciences tend to be more theory driven. Consequently, the literature review is broken into two components. First, we consider how multi-scale modeling is handled in the physical sciences including physics, chemistry, biology, and engineering. Second, we consider how unintended consequences are detected in the social sciences. In the social sciences, the challenge is that there are often so many different abstractions that could be applicable that the notion of organizing them by scale becomes meaningless.

It should be noted that while the physical sciences and social sciences are quite different in terms of terminology and approach, at an abstract level, they are quite similar in intent. Consequently, the increasing prevalence of multi-modeling may end up merging the two approaches in the long run. However, in the short run, the challenge of overcoming these differences remains.

5.1   MULTI-SCALE MODELING IN THE PHYSICAL SCIENCES

Generally speaking, models based on well-established theories exist in different domains. As models, they represent the observed phenomena in an incomplete way – they are not the phenomena. The main assumption behind multi-scale modeling is that by putting these individual representations together, we are working towards a more complete and accurate representation of the phenomena of interest. This means being able to understand the transitions between existing theories and, between models.

On a more practical level, the use of multi-scale modeling seems appropriate to whenever *computational bottlenecks* associated with the growing size of the problem arises (Brandt 2002). For instance, if the computational cost increases significantly with the number of variables or, when the number of variables is so large that linear-scaling algorithms would be very expensive. The low-level resolution of most variables also adds to these bottlenecks.

It is important to review and synthesize the literature on multi-scale modeling as it faces similar challenges albeit in different domains. The focus is on natural sciences and engineering work that provides relevant information on the topic, and, on modeling applications that face major roadblocks due to multi-scale needs. It is organized as follows: after a brief description of different applications of multi-scale modeling is provided, important practical questions are covered. Specifically, we aim to understand how researchers select and couple stand-alone models and prevent model overlap and, validate the resulting multi-scale model.

5.1.1   MULTISCALE MODELING APPLICATIONS

In Physics

A classic example of a scientific roadblock due to multi-scale needs is in physics. Quantum theory works remarkably well in all practical applications (Zurek 2002). States of quantum systems evolve according to the *Schrödinger* equation. Given the initial state, the universe evolves to a state of many alternatives – superposition[1] - never seen to coexist in the world. Everyday objects are expected to obey to quantum mechanics, and their behavior described by the Schrödinger equation. After all, objects are collections of atoms. Yet, they seem to obey to Newton's law instead (Bhattacharya et al 2004). As if classical dynamics emerges in a quantum world. This is the quantum-to-classical transition problem and it represents an example of a multi-scale modeling problem in physics.

Saying quantum-to-classical transition almost implies the existence of a distinct border that separates the applicability of both theories – an important property of a non-overlapping multi-scale model. However, there is no evidence of a border at which the Schrödinger equation would fail (Zurek 2002). There is however, a key aspect to the problem: macroscopic systems are never isolated from their environment. Therefore, their behavior cannot follow the Schrödinger equation as it only applies to closed systems. Macroscopic systems experience what is known as *decoherence* or, a loss of quantum coherence into the environment. The environment induces a *super-selection rule* that prevents specific superposition from being observed. Consequently, only states that resist to this process can eventually become classical.

Decoherence as a concept sets the desired border between the quantum and classical theories. It also justifies the emergence of classical behavior from a quantum model. But how does classicality emerge from a quantum model? Quantum measurements record the potential states of a quantum system. A density matrix[2] describes the probability distribution over the alternative states. A reduction of the state vector takes the pure-state density matrix and cancels the off-diagonal terms that represent purely quantum correlations[3]. The reduced density matrix with only classical correlations emerges. The coefficients of the matrix can now be interpreted as classical probabilities (Zurek 2002). Important to note that reduction of the state vector reduces the information available to the observer. It may also exclude outcomes that are to become classical and, the initial conditions required to predict future states.

It is believed that decoherence and quantum-to-classical transition result from the interaction of a system with its environment. These considerations are based on a specific model - a particle in a heat bath of harmonic oscillators –, which is a reasonable approximate model for more complicated systems (Zurek 2002). Physicists continue to work towards a single multi-scale model (and theory) that explains the emergence of classical mechanics in a quantum world for a wider range of phenomena. There seems to be little space for questions on the stand-alone model selection. Both theories have existed for many years and, have been the subject of experimental scrutiny. New data will lead to new assumptions. Experimental results

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[1] Superposition is the ability of an atom to be in more than one quantum state at the same time.
[2] A density matrix is the analogue to phase-space probability measure (position and momentum) in classical mechanics.
[3] Purely quantum correlations are correlations impossible to achieve when modeling a system with classical mechanics.

might eventually confirm or contradict these assumptions. Anyway, any conclusion on a new multi-scale theory will be based on observation. It seems that until then, we must use one theory or the other to explain the same physical phenomena but at different scales.

In Biology

Cancer is a group of diseases characterized by uncontrolled cell growth and tissue invasion (Deisboeck et al 2011). To model the different carcinogenesis phases from initiation to metastasis a multitude of multi-scale processes must be considered. The use of multi-scale modeling appears as a natural approach. The assumption is that multi-scale models have the potential to refine the existing hypotheses, focus experiments and, improve predictions. Thereafter, improved predictions help in the development of new cancer drugs and treatments. Some studies have been successful in establishing a mechanistic link between some of the processes at different biological levels that contribute to the different carcinogenesis phases (Deisboeck et al 2011). We highlight two of these studies next.

The first study considers how abnormal cell signaling at the molecular level triggers oncogenic transformations. Briefly, the Epidermal Growth Factor[4] (EGF) binds to the Epidermal Growth Factor Receptor[5] (EGFR) and causes cells to grow and differentiate. The EGFR is found at exceptional high levels on the surface of many types of cancer cells. In the presence of the EGF, these cells may divide disproportionately. Abnormal activation of signaling pathways can result in cancer initiation and progression. To model how modified signaling caused by mutations in the EGFR triggers oncogenic transformations, researchers have focused on the simulation of protein structure and protein-ligand interactions, protein intramolecular large-scale motion and protein-membrane interactions and, signal transduction (Liu et al 2007). The spatial and temporal scales of these simulations range from approximately 10^{-10} meters and 10^{-15} seconds to roughly 10^{-6} meters and 10^{0} seconds. The choices for the stand-alone models are molecular dynamics, free energy docking, generalized Langevin dynamics, kinetic Monte Carlo and transient system dynamics. We assume that these are standard model choices for the simulations in question as no justification on model choice was provided. Likewise, no detailed explanation was offered in terms of a general model coupling strategy - just that the individual models were coupled via their inputs and outputs ports. We presume that it followed a somewhat trial and error coupling process. We justify our assumption based on the fact that the study emphasizes the consistency between the multi-scale simulation results and the experimental observations (Liu et al 2007).

The second study considers human brain cancer in specific. Human brain cancer cells proliferate *or* migrate but do not exhibit both phenotypes simultaneously. Experimental evidence shows that a molecular switch operates between cellular proliferation and migration in highly malignant brain tumor cells. The exact molecular mechanism that triggers the phenotypic switch has not been determined yet. A multi-scale attempt to establish such mechanism incorporates a gene-protein decision network into a multi-scale, agent-based model to simulate

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[4] Epidermal growth factor is a protein made by cells and some types of tumors.
[5] Epidermal growth factor receptor is a protein found on the surface of some cells.

the division between cell migration and proliferation and, tumor growth across different orders of magnitude (Athale et al 2005). Cancer cells are modeled as autonomous agents consisting of sub-cellular sites: nucleus, cytoplasm and membrane. These sites are further decomposed into sub-sites that contain all the molecules in the EGFR signaling network. Mass balance reactions and reactions determined by the interaction network regulate the flow of molecules from one sub-site to another. Ordinary differential equations are used to represent the molecular concentration over time. To determine whether a cell should migrate or not, a phenotypic decision threshold is established and the migratory potential for each cell is determined. The simulation results show that cell proliferation or migration impacts cancer expansion as a whole. It also highlights experimentally testable hypotheses on the sub-cellular level. Important to note that the authors of the study suggest that it is the comparison between the multi-scale simulation results and experimental data that paves the road for biological and clinical discoveries.

To conclude this subsection, we highlight a third multi-scale study on the development and prevention of in-stent restenosis. Stenosis is an abnormal narrowing in a blood vessel specially a coronary artery. Current interventions include stent-assisted balloon angioplasty where a small, tubular mesh tube – stent – is deployed at the site of the stenosis and acts as a mechanical structure that compresses the plaque and reduces the changes of vessel collapse (Tahir et al 2011). In-stent restenosis is the recurrence of stenosis after the surgical intervention (i.e. stent deployment). A sequence of multi-scale processes takes place in response to arterial wall damage: local coagulation (thrombosis) that progresses to an inflammatory stage, granulation tissue deployment, smooth cell proliferation, extracellular matrix deposition and remodeling of the neointima (Evans et al 2008). To understand how these processes interact across scales researchers have used a scale separation map (i.e. a graphical representation along different scales). The availability of quantitative data on the spatial and temporal characteristics of the processes is a requirement to build the map.

The in-stent restenosis problem has been modeled in the following multi-scale fashion: it couples a lattice Boltzmann bulk flow solver for the blood flow, an agent-based model for the smooth muscle cell dynamics, and a Finite Difference model for the drug diffusion from the stent and within the cellular tissue (Caiazzo et al 2011). A kernel simulates the deployment of the stent into the cellular tissue and generates the initial conditions. The coupling between the individual models is accomplished via conduits and mappers (Chopard et al 2014). A conduit is a one-way, point-to-point communication that, in this case, converts the positions and radii of cell agents (smooth muscle cell model) into a computational mesh[6] for the flow solver, which is decomposed into fluid and solid nodes (Caiazzo et al 2011). Another conduit converts the same positions and radii into a computational mesh for the drug diffusion solver. Mappers are multi-port data transformation agents[7] that, in this particular application, take the output of the bulk flow solver, of the drug diffusion model, and the present cell configuration to compute the

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[6] A mesh is a discretization of a geometric domain into small and simples shapes such as triangles for 2D and tetrahedral for 3D.

[7] Multi-port data transformation agents combine inputs from multiple conduits and produce multiple outputs.

shear stress on each cell. Similarly to the development of the scale separation map, quantitative data also informs the multi-scale coupling required.

In Chemistry

Two examples from the literature are included here: a homogeneous-heterogeneous chemical reactor model and a hybrid multi-zonal/computational fluid dynamics model of chemical process equipment (Vlachos 1997; Bezzo & Macchietto 2004; Yang & Marquardt 2009).

Homogeneous and heterogeneous processes are frequent in many areas such as catalysis, electrochemistry and corrosion (Vlachos 1997). Some of these processes include the transport of reactants and products in a fluid boundary layer, homogeneous reactions in the fluid phase and, heterogeneous reactions on a surface. Consider, for example, a model of a homogeneous-heterogeneous chemical reactor (Vlachos 1997). The reactor model includes the homogeneous bulk fluid phase and the heterogeneous solid catalyst surface – a partially overlapping decomposition. Absorption, reaction, and desorption of molecules occur at the solid surface. The reactants of the surface reaction in the fluid phase diffuse towards the solid surface. In the opposite way, the products of the surface reactor in the solid surface diffuse into the bulk fluid phase (Yang & Marquardt 2009). In order to generate necessary kinetics information the surface can be decomposed into a molecular lattice.

Hybrid multi-zonal/computational fluid dynamics models are appropriate to model chemical process equipment (Yang & Marquardt 2009). The goal is to decompose the system into different scales in order to simplify computations. Consider a piece of chemical equipment. As a first step, the equipment is decomposed into a number of zones each of which is characterized by a number of variables such as temperature, pressure, etc. To show the heterogeneity of the overall space, these variables have distinct values in different zones. The zone-variable assignment precedes a further decomposition of the zones into cells. The cells also have their own set of variables; however, these variables are constrained by the ones at the zone level. Precision is the main driver behind the decomposition process: whenever the phenomena to be modeled require accurate representation, the decomposition continues down to the cell level. For phenomena that require a lesser precise representation, the reduction to zones suffices. The multi-zonal model maps the overall space and it is independent of the model for each zone. Rather, it is topologically defined with respect to the interfaces that connect the zones (Bezzo & Macchietto 2004). The characterization of the flux of material between zones and the properties that result from fluid mechanical mixing processes are used to determine the coupling scheme. The properties can either be determined from the computational fluid dynamics models or, if required by these models, determined by the multi-zonal model.

In Material Sciences

In materials sciences, it is common to distinguish between different length scales: the atomic scale, the microscopic scale, the mesoscopic scale and, the macroscopic scale. The main players at each of the scales are electrons, atoms, lattice defects (such as dislocations and grain boundaries) and, continuum fields (such as density, velocity, temperature, displacement and

stress fields), respectively (Lu & Kaxiras 2004). Well-established and efficient computational approaches that model phenomena at each scale have been developed over the years. Individually, neither approach suffices to describe multi-scale phenomena. For example, a full atomistic description of material defects alone does not describe the observed macroscopic behavior; higher scale defect interactions do (Curtin & Miller 2003). In fact, material sciences applications are *"hitting the bounds of single-scale models in both time and length scales"* (Germann & Randles 2012). And so, the challenge in material sciences simulation becomes how to combine the available stand-alone models to tentatively tackle unanswered questions in the field.

Conceptually, two multi-scale approaches in material sciences can be envisioned: a sequential approach or a concurrent approach (or both simultaneously) (Lu & Kaxiras 2004). The sequential approach does not couple individual models directly but passes critical information such as material properties from atomistic models to continuum ones. The concurrent approach couples atomistic and continuum models explicitly, which allows for an atomistic description of critical regions and a coarser description of the more uniform regions away from the critical ones (Miller & Tadmor 2009). The goal of any of the approaches is to predict the performance and behavior of materials across space and time scales and to make the best compromise between accuracy, efficiency and, realistic description. To illustrate both strategies, consider the Peierls-Nabarro model of dislocations and the macroscopic-atomistic *Ab initio* dynamics approach (Lu & Kaxiras 2004).

Dislocations are an important concept in the understanding of the mechanicals properties of crystalline solids (Lu & Kaxiras 2004). Continuum elasticity theory explains the long-range elastic strain of a dislocation beyond a few lattice spacings. In close proximity to the dislocation core such explanation falls apart. The Peierls-Nabarro model of dislocations addresses this problem by incorporating a discrete dislocation core structure into a continuum framework. To illustrate it, consider a solid with an edge dislocation in the middle i.e. two elastic half-spaces linked by atomic forces across a common interface. The goal of the Peierls-Nabarro model is to compute the slip distribution[8] on the interface that minimizes the total energy (Lu & Kaxiras 2004). To do so, the elastic energy that is stored in both half-spaces due to the dislocation and the nonlinear potential energy that results from atomistic interactions across the interface must be determined (as these contribute to the total energy). As previously mentioned, elasticity theory determines fairly well the elastic energy in both half-spaces. The limitation arises at the interface. Classical interatomic potentials (or, alternatively, *ab initio* calculations[9]) are used to determine the potential energy due to the atomistic interactions. This atomistic information feeds into the coarse-grained continuum framework, making for a sequential multi-scale approach to the dislocation problem.

Unlike dislocation, the study of fracture dynamics is better approached with a concurrent strategy (Lu & Kaxiras 2004). The reason is that fracture phenomena result from dynamic

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[8] Slip distribution (or relative displacement) is a measure of the misfit across the interface and it characterizes the dislocation.
[9] *Ab initio* calculations are calculations from basic and well-established laws of nature.

interactions between multi-scale processes, which contribute to the total fracture energy. Consider the macroscopic-atomistic *Ab initio* dynamics approach applied to the dynamical fracture process in Si (brittle material). At the crack tip region, atomic bonds break and form; around the crack tip region, atomic bonds do not break but there are significant strain gradients; at the far-field region, atomic displacements and strain gradients are small. At each of the regions, well-established and tested methods apply. Specifically, the macroscopic-atomistic *Ab initio* dynamics approach links a quantum-mechanical tight-binding approximation method to a classical molecular dynamics method to a continuum finite element method, respectively. In between the regions, coupling or handshaking algorithms tackle the transitions. For the finite element - molecular dynamics transition, the algorithm scales down the finite element mesh size to atomic dimensions (or expands it if in the opposite direction). For the molecular dynamics – tight-binding transition, there are fictitious atoms situated directly on the top of the atoms on the molecular dynamics region. On one side of the interface, the bonds to an atom are deduced from the tight-binding Hamiltonian; on the other side, the bonds are derived from the interatomic potential of the molecular dynamics simulation (Lu & Kaxiras 2004).

5.1.2 MULTI-SCALE MATHEMATICS

The previous section illustrates some of the scientific roadblocks due to multi-scale needs. These are domain- or application-driven needs and can be summed up to the integration of heterogeneous models and data that describe multi-scale phenomena of interest. Great complexity results from the many variables and interactions between heterogeneous models and data. Some studies have demonstrated that scale-born complexities can be overcome or, reduced, by multi-scale[10] algorithms (Dolbow et al 2004). This section provides an overview of some of these algorithms. Fundamental to most algorithms are mathematical subjects such as error estimation methods (to estimate error propagation across models and scales which can result from model mismatch and the coupling process for example), uncertainty quantification methods (to characterize and quantify sources of uncertainty and to, together with error estimates, identify the proper scale resolutions in adaptive methods and obtain information on the model solutions and their reliability), inverse and optimization methods (to identify model parameters and control mechanisms) and, dimensional reduction methods (to simplify models with high-dimensional state or input parameter spaces to essential dimensions and modes – reduction in the number of degrees of freedom) (Dolbow et al 2004). These topics will not be addressed in detail here.

Multiresolution methods

The goal of multiresolution methods is to decompose objects into terms resolving different scales or resolutions for the purpose of analysis, approximation, compression or processing (Kunoth 2015). The objects can be given explicitly in the form of, for example, time series or image data, or implicitly as solutions of partial differential equations. Consider, for example, a univariate function f that exists on a finite interval $[0, T] \subset \mathbb{R}$ and that describes a given

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[10] Multi-scale or multi-resolution or multi-level or multi-grid algorithms.

object. The goal of a multiresolution method is to find a decomposition $f(t)$ for j scales or resolutions:

$$f(t) = \sum_{j=0}^{\infty} g_j(t), t \in [0,T], j \in \mathbb{N}$$

An example of a classical decomposition is the Fourier analysis (Kunoth 2015). Fourier analysis converts signals from their original domain, oftentimes time or space, to a representation in the frequency domain (and vice versa). In this case, the multiscale components are of the form

$$g_j(t) = a_j \exp(iw_j t)$$

where w_j are the frequencies and a_j are the constant amplitudes to be determined from f using, for instance, the Fourier transform[11]. Note that, in this particular example, the multiscale components g_j are of a specific form and all are of the same format.

Some multiresolution methods include multiresolution analysis and multiscale geometric analysis, and multigrid and algebraic multigrid (Dolbow et al 2004).

Multiresolution analysis and multiscale geometric analysis

Given a basis function φ in $L^2(\mathbb{R})$, we consider the scales and translations of φ: φ_k^j for j and k in $\mathbb{Z}$. The subset of $L^2(\mathbb{R})$ describable by a linear combination of the set of functions φ_k^j can be written as:

$$V_j = \overline{span\left\{\varphi_k^j \middle| k \in \mathbb{Z}\right\}}$$

If every $f \in L^2(\mathbb{R})$ can be arbitrarily correctly approximated by the set of φ_k^j and φ fulfills a refinement equation, we say that φ or the V_j's build a multiresolution analysis (Schneider and Krüger, 2007). Assume that φ fulfills a refinement equation, $V_j \subset V_{j+1}$ for every $j \in \mathbb{Z}$. As such, there is the orthogonal space W_j of V_j in V_{j+1} and:

$$V_j \oplus W_j = V_{j+1}$$

W_j is called the detail space or the wavelet[12] space for V_j. So, given a level J we want to approximate, we have:

$$V_J = V_{J-1} \oplus W_{J-1}$$

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[11] The Fourier transform decomposes a function of time (signal) into the frequencies that make it up.
[12] A wavelet is a short wavelike function that can be scaled and translated.

$$= V_{J-2} \oplus W_{J-2} \oplus W_{J-1}$$

$$= \cdots$$

$$= V_0 \oplus \bigoplus\nolimits_{j=0}^{J-1} W_j$$

Multiresolution expansion based on wavelets has a great number of successful applications in data compression and noise removal (Donoho 2002). The rapid increase in new data sources, each different from the other, sustains the need for expansions that uniquely adapt to each data type. Wavelet analysis is exceptional for representing smooth data containing point singularities but not singularities of intermediate dimensions, which in some cases represent important features. This suggests that in higher dimensions, wavelets do not suffice and there is a need for a geometric multiscale analysis. Previous attempts in this direction discuss two approaches to geometric multiscale analysis: a directional wavelet transform based on parabolic dilations and, analysis via anistropic strips (Donoho 2002).

<u>Multigrid and algebraic multigrid methods</u>

Mathematical models in science and engineering make extensive use of differential equations to solve problems (Wesseling 1995). Multigrid methods target the algorithmic efficiency to solve differential equations. It usually starts with the application of a smoother (or relaxation method), which is often a simple iterative method such as the Jacobi or Gauss-Seidel method (Falgout 2006). The goal is to have a smooth error in a few iterations and then to move to a coarser grid on which the remaining error can be removed. The steps of the coarse-grid correction process are 1) to transfer information to a coarser grid, 2) solve a coarse-grid system of equations and, 3) transfer the solution back to the fine grid. To illustrate, consider we want to solve for:

$$A_h \boldsymbol{u} = \boldsymbol{b}$$

where A_h is the (original) real n x n matrix on fine mesh and $\boldsymbol{u}$ and $\boldsymbol{b}$ are vectors in $\mathbb{R}^n$. The key components to multigrid are a restriction matrix R and an interpolation matrix I that change the grids (Strang 2006):

1. A restriction matrix R transfers vectors from the fine to the coarse grid

2. The return to the fine grid is done by an interpolation matrix $I = I_{2h}^h$

3. The original matrix A_h on the fine grid is approximated by $A_{2h} = RA_hI$

Note the use of a convenient ratio 2 for grid spacing ($h, 2h \dots$). Despite the fact that it is possible to have different spacing, for example h_x and h_y in two dimensions, having a single mesh width h is easier to visualize (Strang 2006).

The algebraic multigrid method solves linear systems based on the same multigrid concepts just described: smoothing and coarse-grid correction. The difference is that algebraic multigrid does not require explicit knowledge of the problem geometry. Instead, it is a matrix-based method. To illustrate, consider we want to solve for:

$$A\boldsymbol{u} = \boldsymbol{b}$$

where A is the (original) real n x n matrix and $\boldsymbol{u}$ and $\boldsymbol{b}$ are vectors in $\mathbb{R}^n$. In linear algebra, the operators that transfer information between the fine and coarse grids are denoted as the vector space $\mathbb{R}^n$ and the lower-dimensional (coarser) vector space $\mathbb{R}^{n_c}$. Also, the map from the coarse to the fine grid (interpolation) is denoted as the n x n_c matrix $P: \mathbb{R}^{n_c} \rightarrow \mathbb{R}^n$ and the map from the fine to the coarse grid (restriction) is the transpose of interpolation, P^T. The two-grid method for solving $A\boldsymbol{u} = \boldsymbol{b}$ is next described (Falgout 2006):

1. *Do v_1 smoothing steps on $A\boldsymbol{u} = \boldsymbol{b}$*

2. *Compute residual $\boldsymbol{r} = \boldsymbol{b} - A\boldsymbol{u} = Ae$*

3. *Solve $A_c e_c = P^T \boldsymbol{r}$*

4. *Correct $\boldsymbol{u} \leftarrow \boldsymbol{u} + P e_c$*

5. *Do v_2 smoothing steps on $A\boldsymbol{u} = \boldsymbol{b}$*

A few remarks about the above algorithm (Falgout 2006). Error e, is the difference between the precise solution and the current iterate: $e = A^{-1}\mathbf{b} - \mathbf{u}.$ In 3., we solve for e_c, the coarse approximation to error e (in practice, the coarse system is solved by recursively re-applying the method). The most popular approach to determine the coarse system A_c is to use the Galerkin operator, $A_c = P^T AP$.

Hybrid methods

The goal of hybrid methods is to couple models and numerical representations across different scales and over contiguous domains (Dolbow et al 2004). The stand-alone models are not required to use a multi-resolution method. The exchange of information between these models has to accommodate for potential discrete to continuum and stochastic to deterministic information type differences. The coupling strategy in hybrid methods highly depends on information concerning error and uncertainty. This information is fundamental to adaptively choose between the available algorithms and parameters during runtime, i.e. to select the coupling form and strength and, to highlight space and time regions where better descriptions are necessary. Some hybrid methods include partitioned-domain methods, hierarchical methods, and sequential and concurrent coupling methods (Dolbow et al 2004).

Partitioned-domain methods

Partitioned-domain methods rely on the atomistic and continuum partitioning of models. Fundamental to this type of partitioning is the computation of the total energy of a system as a function of the degrees of freedom, i.e. the atoms or the finite element nodal position (Curtin & Miller 2003). To determine energies and forces on individual atoms, it is common to use classical interatomic potentials, in which the total atomic energy E^a can be obtained as:

$$E^a = \sum_i E_i$$

where E_i is the energy of the i th atom. Classical interatomic potentials are mostly used in the embedded-atom method or the Stillinger-Weber framework (Curtin & Miller 2003). According to the embedded-atom method, the energy of an atom i is given by:

$$E_i = F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j\neq i} V_{ij}(r_{ij})$$

where F_i is an electron-density dependent embedding energy, V_{ij} is a pair potential between atom i and the neighboring atom j and, r_{ij} is the interatomic distance (Curtin & Miller 2003). The electron density at atom i, denoted as $\bar{\rho}_i$, is the superposition of density contributions from each one of the ρ_j neighbors:

$$\bar{\rho}_i = \sum_{j\neq i} \rho_j(r_{ij})$$

According to the Stillinger-Weber framework, the energy of an atom i can be obtained as:

$$E_i = \frac{1}{2}\sum_{j\neq i} V_{ij}(\boldsymbol{r_{ij}}) + \frac{1}{6}\sum_{j\neq i}\sum_{k\neq(i,j)} V_{ijk}(\boldsymbol{r_{ij}}, \boldsymbol{r_{ik}})$$

where V_{ijk} is the three-body potential and $\boldsymbol{r}_{ij}$ is the vector from atom i to neighbor atom j (Curtin & Miller 2003). When one atom is displaced in an atomistic simulation, the interaction energies are assumed to extend within the range R_{cut} along the neighbor distances. In the absence of externally applied forces, the forces on atom i can be obtained as:

$$f_i = -\frac{\partial E^a(\{\boldsymbol{r}_1 \dots \boldsymbol{r}_N\})}{\partial \boldsymbol{r}_i}$$

The total energy and the forces on each atom allow us to determine the equilibrium atomic configuration as a function of applied forces and imposed displacement on the atoms.

Moving to the continuum side of the partitioning, continuum mechanics assumes that a strain energy density functional W exists for a material and, the energy in an incremental volume $d\boldsymbol{V}$ around point $\boldsymbol{X}$ is $W(\boldsymbol{X})d\boldsymbol{V}$ (Curtin & Miller 2003). The overall potential energy of the material, E^c is obtained as the integral over the volume Ω of the body:

$$E^c = \int_\Omega W(\boldsymbol{X})\mathrm{d}\boldsymbol{V}$$

To determine the equilibrium strain field related to applied forces and displacements in the body, the overall potential energy E^c must be minimized (Curtin & Miller 2003). A common method for the minimization is the finite elements (FE) method. The idea is to determine the displacements $U_j = \mathrm{u}(X_j)$ at a set of points X_j (the nodes j). Predetermined interpolation or shape functions are used to determine the displacements at locations away from the nodes. Elements result from defining polyhedral regions with the nodes at vertices so that the space is covered by elements. The total energy of the continuum region can then be obtained as the sum over the elements μ:

$$E^c = \int_\Omega W\mathrm{d}V = \sum_\mu^{N_e} E_\mu$$

$$E_\mu = \int_{\Omega_\mu} W(X)\mathrm{d}V$$

where N_e is the number of elements in the region and Ω_μ the volume of element μ. The strain energy density functional W depends on the deformation gradient $\boldsymbol{F}$. Changes in the displacement node i trigger changes in the deformation gradients $\boldsymbol{F}$ of all the elements in which node i is contained and, therefore, a change in the total energy. The energies of the other elements are assumed to remain the same (Curtin & Miller 2003).

A critical aspect of partitioned-domain methods is the transition region between the atomistic and continuum partitioning. There is no unified and formal theory of the transition that establishes quantifiable error bounds (Curtin & Miller 2003). There are however, different ways to handle it. For example, Miller and Tadmor (2009) consider the idealized partitioning of a domain problem into B[A] and B[C] that represent the atomistic and continuum partitions of the problem, respectively. The interface between regions B[A] and B[C] is denoted as B[I] across which compatibility and equilibrium are imposed.

A common strategy to bridge regions B[A] and B[C] is to divide the interface region B[I] into the *"handshake region"* B[H] and, the *"padding region"* B[P]. B[H] is both atomistic and continuum. B[P] is continuum but it is used to create atoms that generate the boundary conditions to the atoms in regions B[A] and B[H] (Miller & Tadmor 2009). Such requirement results from the nonlocal nature of atomic bonds. The range of these atomic interactions, R_{cut}, determines the thickness of the padding region. The continuous displacement fields at the position of the padding atoms in the padding region determine their motion. A variation to this interface is to eliminate the handshake region.

A large number of partitioned-domain methods have been proposed in the literature (Miller & Tadmor 2009). These are the quasicontinuum method, the coupling of length scales method,

the bridging domain method, the bridging scale method, the composite grid atomistic continuum method, the cluster-energy quasicontinuum method, the ghost-force corrected quasicontinuum method, the ghost-force corrected cluster-energy quasicontinuum method, the finite element/atomistics method, the coupled atomistics and discrete dislocations method, the hybrid simulation method, the concurrent AtC coupling method, the ghost-force corrected concurrent AtC coupling method, and the cluster-force quasicontinuum method. Although theoretically different, and with the exception of the coarse-grain molecular dynamics method, these methods are similar at the level of implementation (Miller & Tadmor 2009). Differences exist in terms of the governing formulation, the coupling boundary conditions, the handshake region, and the treatment of the continuum. A thorough comparison of these methods in terms of accuracy and efficiency of the coupling led to a unified framework where the different methods can be represented as special cases (Miller & Tadmor 2009).

Hierarchical methods

In hierarchical methods, numerical techniques are independently employed at different length scales. A bridging methodology such as statistical analysis methods, homogenization techniques, or optimization methods can then be used to identify the relevant cause-and-effect relations at the lower scale and their impact at the higher scale (Horstemeyer 2009). An example of a top-down hierarchical approach is the use of thermodynamically constrained internal state variables at the macroscale that reach down and receive information from multiple subscales. This way, the internal state variables macroscopically average the details of the microscopic configurations and capture their effects but not the causes at the local levels. The assumption is that the complete microscopic arrangement is not required as long as the macroscale internal state variables representation is complete (Horstemeyer 2009).

Sequential versus concurrent coupling

The goal of sequential coupling methods is to obtain a macroscopic model from which the macroscopic behavior of systems can be analyzed under different conditions (Weinan 2011). Microscopic models precompute or tabulate some of the functions or parameters that are inputs to the macroscopic models (can too be interpolated). An example of sequential coupling, also called precomputing, microscopically informed modeling, or parameter passing, is found in gas dynamics. Kinetic theory can be used to precompute the equation of state, which is stored in a look-up table and later used in Euler's equations of gas dynamics to simulate gas flow under different conditions. Other examples include the study of macroscopic properties of fluids and solids that use parameters obtained successively from quantum mechanics models. A sequential approach is not feasible when the unknown components of the macroscopic model (parameters or functions) depend on many variables. For example, in molecular dynamics theory, the interatomic forces depend on the positions of all the atoms in the system. However, it is impractical to precompute these forces as functions of the atomic position for more than ten atoms (Weinan 2011). Concurrent coupling offers an alternative in which the unknown components are obtained *"on the fly"* as the computation evolves. For most numerical (concurrent) methods, the macroscale quantities of interest are obtained from appropriate

microscale models and not from ad hoc macroscale models. Oftentimes, the technicalities seen in a sequential or concurrent approach are comparable. The right approach to use depends on how much it is known about the macroscale process.

Heterogeneous multiscale method

The heterogeneous multi-scale method is a top-down approach that relies on the efficient coupling between macroscopic and microscopic models (Weinan et al 2007). The available macroscopic information about the process under consideration (i.e. macroscopic variables and structure) is first entered in the macroscopic model. Examples of information include variational structure, conservation laws, diffusion processes, etc. The microscale models have to be consistent with the just identified macroscale structure. In the context of fluids and solids, for instance, this means to derive conservation laws from molecular dynamics and to express the stress in atomistic variables.

The general setting can be described as follows (Weinan et al 2007). Consider a microscopic system and a microscale model, which can be abstractly described as:

$$f(u, b) = 0$$

where u is the system's state variable and b represent the auxiliary conditions of the problem (e.g. initial and boundary conditions). The microscopic details of u are of no interest; instead, we want to perceive the macroscopic state of the system, U, which satisfies some abstract macroscopic equation:

$$F(U, D) = 0$$

where D represents the necessary macroscopic data for the macroscopic model to be complete. Assume that the compression operator Q maps u to U, and an operator R reconstructs u from U:

$$Qu = U$$

$$RU = u$$

and that $QR = I$ is satisfied (I stands for the identity operator). The purpose of the heterogeneous multiscale method is to determine U using the abstract macroscopic equation F and the microscale model. Despite the incompleteness of the macroscopic model, a macroscopic solver must be selected - all information on the form of F is used to do so. To estimate the required macroscale data, a series of constrained microscale simulations consistent with the local macroscopic state, i.e. $b = b(U)$ follow and, the microscopically generated data is next used to extract the required macroscale data. Data estimation can be conducted *"on the fly"* or in a pre-processing step (likewise in the concurrent and sequential coupling methods, respectively). There is no direct communication between the microscale models; all communications are performed through the macroscale solver (Weinan et al 2007).

Adaptive methods

The goal of adaptive methods is to minimize the error and uncertainty in simulation and data representation (Dolbow et al 2004). There is a trade-off between the efficiency of a coarse scale simulation and the precision of a detailed one. The computational effort is locally adjusted to keep a uniform level of precision throughout the problem domain (Colella, n.d.). While adaptive methods, in specific the adaptive mesh and algorithm refinement, may look similar to hybrid methods, there are fundamental differences between them (Garcia et al 1999). For instance, the adaptive mesh and refinement algorithm explicitly works as a multi-level method that simulates systems whose length scales are of considerable orders of magnitude. Furthermore, it is fully three-dimensional whereas some hybrid methods are limited to the simulation of one- or two-dimensional problems.

Adaptive mesh refinement

Adaptive mesh refinement is a numerical method for solving a class of partial differential equations in one or more dimensions (Berger & Colella 1989). It hinges on a series of embedded, logically rectangular grids on which the partial differential equation is discretized. An error estimation procedure based on user-specified criteria determines where additional refinement is necessary (Garcia et al 1999). Grid generation procedures dynamically create or eliminate finer grid patches as resolution requirements vary. To illustrate, consider a sequence of levels $l = 1, \ldots, l_{max}$ and define a grid G_l:

$$G_l = \bigcup_k G_{l,k}$$

where grid $G_{l,k}$ has mesh spacing h_l. Each grid is a subset of the rectangular discretization of the entire space (Berger & Colella 1989). Overlapping grids at the same level l are possible; yet, the discrete solution must be independent from the decomposition of level l. Grids at different levels must be properly embedded. Specifically, a fine grid starts and ends at the corner of a cell of the next coarser grid and there must be at least one level $l - 1$ cell in some level $l - 1$ grid that separates a grid cell at the coarser grid l from a cell at the finer grid $l - 2$ in the north, south, east, and west directions (Berger & Colella 1989). The exception is when the cell is on the border of the physical boundary of the domain.

Grids with finer mesh width in space will also have smaller mesh width in time (Berger 1982). In other words, refinement is done in both space and time by the same refinement ratio (Berger & Colella 1989). The mesh refinement algorithm includes an error estimation procedure and an integration algorithm. There are three components in the integration algorithm: the actual time integration on each cell (application of finite differences), the error estimation and consecutive grid creation and, the grid-to-grid operations required at each time step (Berger 1982).

Adaptive time-step algorithm

The adaptive time-step algorithm makes use of appropriate time steps based on Courant-Friedrichs-Lewy (CFL) considerations to advance the different levels (Garcia et al 1999). The algorithm carries out operations that advance each level independent of the other levels in the hierarchy – the exception being the operations for the boundary conditions. Finally, a synchronization of the levels takes place: the fine grid is averaged onto the coarse grid and, the difference in flux between the coarse and fine grids (boundary) is corrected (Garcia et al 1999).

Adaptive mesh and algorithm refinement

The adaptive mesh and algorithm refinement uses a particle method to evaluate flux in regions where microscopic resolution is required and a continuum method with variable levels of refinement otherwise (Garcia et al 1999). The algorithmic structure of the adaptive mesh and algorithm refinement method is comparable to that of the adaptive mesh refinement method. The difference is in the use of a direct simulation Monte Carlo calculation to evaluate the finest grid level. There are four main routines that address the interaction between the continuum solver and the direct simulation Monte Carlo region. These routines i) pass the time-interpolated state to the particle buffer cells (buffer cells surround the direct simulation Monte Carlo region), ii) pass the momentum and energy corrections to the direct simulation Monte Carlo region, iii) receive the fluxes stored when particles cross the direct simulation Monte Carlo interface and, iv) receive conserved densities for continuum cells that cover the direct simulation Monte Carlo region (Garcia et al 1999).

Equation-free multi-scale method

The equation-free multi-scale method is designed for systems in which macroscopic evolution equations exist but are not available in a closed form. Modeling through macroscopic equations, if possible, requires assumptions difficult to justify. Instead, fine-scale models are initialized on short time and small length scales to accomplish tasks at a macroscopic level. The method comprises different techniques such as coarse projective integration, gap-tooth scheme and, patch dynamic (Dada & Mendes 2011).

Coarse projective integration

Microscopic simulations are performed and the solutions used to determine the average values of the coarse variables. These, in turn, are used to compute the coarse time derivatives required to extrapolate the coarse variables over larger time steps. The microscopic simulations use initial data that is coherent with the present macro-state.

Gap-tooth scheme

The idea is to cover the space with teeth (small domains over a short time period) and intermediary gaps to approximate the evolution of a macroscopic equation. The simulation of

the microscopic evolution is performed within each tooth. Boundary conditions at the edges of each tooth need to be specified.

Patch dynamic

Patch dynamic is the combination of the coarse projective integration with the gap-tooth scheme.

5.1.3 OTHER METHODS

Multi-scale agent-based modeling method

Multi-scale agent-based modeling models the behavior of autonomous agents – individually or collectively – and their interactions in order to simulate their impact on the overall system. It is object-oriented, rule-based, discrete event and, discrete time (Dada & Mendes 2011).

Complex automata

The method hinges on the idea that systems can be decomposed into N single-scale cellular automata that interact across spatial and temporal scales. The graphical representation of each subsystem and respective scales is frequently done using a scale separation map. The exchange of information across subsystems is achieved through coupling mechanisms such as, the sub-domain coupling and the hierarchical-model coupling. In the former, different models describe neighboring spatial domains (possibly with different resolutions), while in the latter, some parameters of the central model are computed as necessary by lower resolution models (Hoekstra et al 2007).

Multi-scale numerical scheme

The multi-scale numerical scheme aims at finding the numerical solution of bidomain equations. Bidomain equations are a system of elliptic partial differential equation and parabolic partial differential equation, coupled at each point in time by a system of non-linear ordinary differential equations (Whiteley 2008). These equations are frequently used to model cardiac electrophysiology. The multi-scale numerical algorithm assumes that computation at a high resolution is resorted to a very small number of variables that change on a short time-scale and short length-scale. A fine mesh is used to approximate these rapidly varying variables whereas a coarser mesh is used to compute the remaining ones. When required, linear interpolation is used to transfer the slower variables onto the finer mesh.

In situ adaptive tabulation multi-scale approach

The approach focuses on multi-scale problems where a large number of ordinary differential equations with identical initial conditions needs frequent evaluation. Instead of solving for all the equations, previously calculated solutions are stored and used as approximations whenever a new solution with similar initial conditions is needed. These approximations also satisfy a given error tolerance (Dada & Mendes 2011).

5.1.4 Discussion and conclusions

While there are different strategies to multi-scale modeling, the key challenge is how to couple stand-alone models (Weinan et al 2007):

- We can match the models using handshake regions or across interfaces

- We can impose constraints on the micro-scale model to ensure consistency with the local macro state

- We can extract the macro-scale data from the micro-scale simulations

- We can link micro-scale simulations on small boxes to mimic micro-scale simulations over the entire domain

The review of the literature shows a great emphasis on the available theories, research, and models at the different scales but not on the coupling strategy, which is the aspect that is most relevant to this research effort.

As far as selecting the models to be composed, some applications seem to reuse available models while others seem to use whatever models are standard for that scale. Regardless, most of the models have previously been validated. Unfortunately, almost always, no explanation on model selection is given. Particularly relevant to this effort is how overlap among the various models is handled. Not surprisingly, partitioning of the domain space is a way to prevent model overlap, but overlap exists explicitly in some multiscale methods.

Of course, when one creates a multi-scale model validity is an issue. The validity of the stand-alone models does not determine the validity of the multi-scale model. Moreover, it is important to look for contradictions and incompatibilities between the individual models. Some models may be based on theories that are hundreds of years old and have been repeatedly tested, while others may be much more recent and tentative. Consequently, we observe that experiments have been fundamental to validate multi-scale models.

Of course, the critical question is whether these multi-scale modeling techniques can be used to identify unintended consequences. Through the literature, there seemed to there seemed to be an implicit assumption that multi-scale modeling is the path to scientific discovery and engineering design. However, the review shows that the focus of most applications tends to be on prediction that is validated based on comparisons to experimental results. Thus, these multi-scale modeling techniques are effectively forms of interpolation, and discovery is an outcome of exploration and not interpolation.

Our hypothesis is that a lack of a systematic process for component model selection is the reason for this outcome. It is the exploration of alternative model structures that has the potential to identify unintended consequences. When the model selection is either ad hoc or based on standards and then "tuned" to match experimental data, one has effectively removed the ability to generate alternative consequences. Thus, if something unexpected is going to

occur, is going to occur in the experiment. The reason is if the model deviates from the experiment, it is adjusted to match the experiment.

It is also worth noting that when we originally considered this topic in engineering, one approach that seemed relevant was multi-disciplinary optimization (MDO). In fact, some of this literature was discussed in the RT-138 final report (Pennock et al 2016). However, it was realized during the course of the investigation that MDO is a special case of the multi-modeling problem where any overlap issues among the models are tolerable. In the language that will be developed in Section 6, there are either no or one-way transition linkages among the models. Consequently, while these techniques are important to engineering in general, they are less informative for addressing the challenges examined in this study.

5.2   FINDING UNINTENDED CONSEQUENCES IN THE SOCIAL SCIENCES

While there are many possible starting points within social science, it is useful to start with measure theory. We will start the discussion by expanding upon the prominent modeling approaches within psychometrics, econometrics, and to the extent possible sociology. Measure theory paradigms have sub-domains and categories, but we will use latent variable theory (LVT) as it has been identified as useful for cognitive behavioral phenomena. But it is useful to know, that in congruence to much social theory, that the paradigm is embedded in other model paradigms: random control trial, machine learning techniques, and dynamical equilibrium to name some prominent ones. Seeing as there is no 'conscious'-meter or 'economicus'-meter per se, social measure has to constantly assume at least the possibility of latent effects and their effects on potential model transformations.

We review this with two minds within socio-technical enterprises. First being the establishment of latent or relative model phenomena in enterprises establish methods from previous research. The walkthrough below borrows the psychometric perspective as it is presumed this is more useful to make the observable points, so this is then rooted in item response theory language and related formal stances viewing 'technical' aspects as 'items' toward which cognitive actors respond. It is also where the root mathematical measure theory developed, so has embedded the theoretic motivations presumably. Also concerning enterprises, the individual (or small group) behavior is often where the model difficulties occur; for instance reviewed in the previous RT was that higher-order effects occurred when individual drivers acted on a conversing utility curve can be viewed as 'latent'. So then of second mind, is to consider how more generally social sciences differ in their philosophy of science that would be relevant to enterprise systems engineers.

Considered in the methodology, it is hoped that the audience has an appreciation on (linear) algebra and normative statistics. The measure theory portion is based in these maths which should not be new to most modelers, but the observed hypothesis is that there are unique analytic considerations and spatial reasoning than what is traditionally covered. The review

then lists specific methods where could be found, and instead focuses on the theory and intuition underlying the modeling and specifically the approach to error analysis. We refer those interested in specific model classes or exampled uses to the cited works provided and have referred works that inundate the reader with the most broadly referenced works found. So to say, that the references are not central in the sense of seminal but rather of importance by establishing theory or being a meta-review with referenced works themselves.

One impression is that much of the methods are not entirely different in underlying mathematics, but as will be discussed, establishing observed items as a model within the social science purview is often the crux of the analysis. As such the 'language of the social science' is important in maintaining the current referent between model and phenomena and often presented in dualistic, dialectic considerations. Social science cannot always take for granted that symmetry between model objects and their objects of study. So those observations based in mathematical description will try to be faithful to impressed systems language use while using encountered terminology within social science for those observations more firmly rooted there. This said on strong occasion many terms will be synonymous however with the complexity implicit in psycho-social elements noticing the creation of differences should be most attentive.

Of last note, the goal of the overview is reaching the model groupings and observations on theory use to both inform system practitioners and create descriptive constructs to relate the breadth of literature. The write-up sectioning then covers LVT classes by those given by theory development and impressed current usage. Yet take attention that these classes are not per se consistent across social theory sub-disciplines. For instance, the 'machine learning' paradigm uses statistical measures and linear algebraic manipulations, but one might think to class their usages differently. The classes here are those from the Psychometric Society and categorical review papers with some applicable measure examples in Econometrica. (For additional background see (Epstein & Zhang 2001; Ploberger & Phillips 2003; Angeletos & Pavan 2007; Matsuyama 2004; Giraud 2014).) In subsequent sections, these classes are covered more broadly. However here is to explain within one theory area how the epistemic considerations develop and that the epistemic considerations do appear to carry across modeling efforts.

5.2.1 STARTING MODEL SET-UP: ITEM RESPONSE AND THE SINGLE FACTOR MODEL

A fundamental beginning point for creating a variety of complex measures is to explore wanting a simple objective explanation with which to begin future observations; a 'kernel' if one wills. Factor modeling is often traced to Spearman and the venerable intelligence factor (intelligence quotient, IQ) as anyone who has taken standardized testing measures will be familiar. In modern terms, the motivation for an "intelligence" factor might be better termed as a human ability for "anti-entropic" mental capacity, and then quotient is trying to find potential quotient relationships amongst a group. Human abilities generally had been explored within psychology, yet there is conflicting methods problem when measuring human manifested phenomena that must be crossed. Comparing to a physical system, one would like to create something similar to a thermodynamics measure by observing directly a variant created by the system (e.g. a

thermometer for thermodynamic temperature), and use statistical inference to obtain objective descriptions.

The question became how does one do this for a 'human measure method' with enough empiricism to replicate measures similar from thermodynamics -> thermometer. Human phenomena was (and perhaps still is) not objectively known enough to establish what could be equivalent of a 'intelligence-meter'; even though at the time an intelligence phenomena was established qualitatively (Cudeck & MacCallum 2012). Particularly then humans exhibit means for discerning other's traits as we are conscious beings, but then one loses the objectivity nicely given by physical meters. Hence a seeming inconsistency in psycho-social measurement that ideal symmetries then trade with objectivity both impacting the ability for model inference.

There is then an ongoing abstraction to split at the beginning as one needs a qualitative description but lacks a sufficient analytical means to objectify this linguistic. Then the question from Spearman became to reason how does one create means to split this difference for particular factoring when the factor is inherently what is now termed 'latent' or 'not directly measurable'. As Bartholomew notes, the original paper spends only an appendix briefing on factor modeling and the rest was determining epistemically how a "General Intelligence" description can be gained from "[generalizing] Sensory Discrimination" (Bartholomew 1995). In Bartholomew's words describing Spearman,

> *"Of more immediate relevance to factor analysis, [Spearman] states what he calls "our general theorem", which is "whenever branches of [cognitive] activity are at all dissimilar, then their correlations with one another appear wholly due to their being all variants wholly saturated with some common fundamental function (or group of function)". He distinguishes this central Function from "specific factors seem in every instance new and wholly different from that in all others".*

The impression to modelers is to first consider the objects involved and how one can rely on reasonable theorems to relate to our sensory experience. Certainly one can claim any experience is then within purview, but amidst this purview can be a subjective experience and thus induces possible subjectively created phenomena: e.g. placebo effects, self-fulfilling prophecies, unintended consequences, etc. This quickly leads into theory on causality which while applicable is both outside purview and specifically what Spearman and modelers would like to avoid. Spearman's observation was congruent to system modelers' intention in wanting orthogonal measures (his "branches on activity"). The reasoning then is that if these objectively orthogonal measures are then "saturated" with covariates then one can reason that the remaining variant factors is a wholly 'human' or 'social theoretic'. This should prompt modelers that measuring within the social science starts from establishing a reasonable ontology but additionally choosing objects such that one allows this 'saturation effect' to then map to the 'psycho-social' phenomena of interest: not just in choice objects but couching those objects within epistemic type (sensory item, cognitive item, latent personality, etc.) as Spearman notes.

Taking the standardized testing example, many students are familiar with the itemized set up. Individual items with bounded answer set defines a measurement analysis domain (i.e. an answer sheet) paired with an individual amongst a group. This then provides a mapping of an individual or individual group from their responses to a defined objective measure; the initial insight being creation on what now recognized as a measure set (Lebesgue or Borel) per individual and by inverse a measure of items per individuals. Now a trivial difference measure would be to take an individual response compared to the ideal answer set (grading) to create a numerical value to each individual (score) then rank order individuals by comparison to bounded axiomatic set of numbers (students along 0-100 point value).

While this serves as an objective inference on answering, this falls to inconsistency as the 'answer set' is its own item response from other individuals thus being a subjective determination on the measure. The question posed by Spearman was that considering latent effects such as cognition or personality how does one reasonably map the objective score responses to human phenomena that appear to be on 'higher-order' effects, what mathematically are ordinal phenomena. Particularly how to do this given what we would now know as things such as priming, environment, and general bias that others embed within the 'measuring device'. There is then a whole discipline of study that examines the effects within different experimental set-ups (i.e. measuring device configuration) termed experimental theory and experimental design (Shadish et al 2001). For architecture and design disciplines, these later are suggested as primers.

The main contribution that then spawned (latent) factor analysis in the social sciences was to instead think to use regression on the measures then analyze the correlational space for difference measures. In our testing, this would mean regressing the answers across multiple statistical moments: individual scoring, individual scores across items, and items scores across tests. And in doing so gain 'measure sets' again from their correlation matrices. As noted in the previous study (RT-138), the examination on different ordinals and statistical moments were a modeling basis for much of the 'warning signal' literature (Pennock et al 2016), so the basis on LVT has the same shared intuition.

The argument then is that unique internalized factors such as intelligence would show themselves over the course in changes to normalized responses. Defining a human factor as an objective ability answered less by the question "How does this factor present directly from measure?" but "How does this factor present itself nonrandomly over iteration of a measure?". If one is familiar with general intelligence model (g-theory), this is a one factor model ("across item" intelligence) from predefined item response (intelligence test).

Now inferring the measurement can be seen through the partial correlation coefficients (Yule 1897). One can recognize the distance measure form from variables taken from a matrix space on the computed partial correlations. Analyzing the correlation coefficients can show ordering patterns across moment coefficients within linear algebraic representation compared to a hypothesized general factor. This then allows an objective basis to examine more ordinal responses presuming these are expressed across statistical moments.

$$\rho_{xy|z} = \frac{\rho_{xy} - \rho_{xz}\rho_{yz}}{\sqrt{(1 - \rho_{xz})^2(1 - \rho_{yz})^2}}$$

$$\begin{bmatrix} \rho_{xx} & \cdots & \cdots \\ \rho_{xy} & \rho_{yy} & \cdots \\ \rho_{xy} & \rho_{yz} & \rho_{zz} \end{bmatrix}$$

Identifying that there are non-random profiles within the partial correlations in this case between individual answers is then the goal. Of interesting support, there was a competing model using sampling modeling which may be more familiar to those within an informationalist background (Thomson 1950). Even as the underlying sampling model has better correspondence to modern brain functioning (Mackintosh 1998) (what most might recognize as a Bayesian updating), Bartholomew points out that to identify the higher order effects to break our 'inconsistency psychometric problem' using statistical moments is again necessary and then congruent to the Spearman model. Then even across first order response models, this 'intelligence factor' is identified by non-standard jumps in response profiles and recognized by the ability to intake and respond at a statistically higher ordinal; being able to read, respond, iterate over the course of several items, and observable across different first order models. Then when seeking to make a single factor model, the factor variable (IQ) is composed with the correlation variables rather than determining the direct test score model which helps resolve the subjectivity inference problem on the item choice and inference basis. From a modeler's perspective, this would seem to be an inconsistency choice problem on the model basis. In fact by the theorem, the basis algebra is relatively irrelevant comparatively as it is constructed irrespective of first order model choice (still ultimately important as the observable measures still need mapping to a basis algebra). As any choice of a particular model basis still must be broken into an ordinal spacing, the kernel of the analysis is the covariate profile.

From this the general LVT form can be presented. Below the basis for the model estimation which identify general variable objects. This is then presented in a matrix field over the covariate-correlation profiles; presented in expected value form. While additional assumptions are needed for an analytic solution, once can get a general algebraic appreciation from Moustaki et al (2015):

$$x_i = \tau_i + \lambda_i\xi_i + \delta_i$$
$$x = \text{'observed variable'}$$
$$\xi = \text{'common variable' (ie latent factor)}$$
$$\lambda = \text{'factor loading}$$
$$\delta = \text{'unique factor'}$$
$$\tau = \text{'constant factor' (if needed)}$$

$$\sum\theta = \begin{bmatrix} Var(x_i) & \cdots & \cdots \\ Cov(x_{i+1}, x_i) & Var(x_{i+1}) & \cdots \\ \vdots & Cov(x_{i+2}, x_{+1}) & \ddots \end{bmatrix} = \text{"Covariate Matrix"}$$

$$Var(x_i) = Cov(x_i, x_i) = E[(x_i - E(x_i))^2]$$

$$Cov(x_{i+1}, x_i) = E(x_i, x_{i+1}) - E(x_i)E(x_{i+1})$$

Now to close this first section, the use of strict assumptions for analytic solution and then statistical inference is a needed constraint. Specific assumptions and convergence estimations are covered in later sections, yet the generalized incompleteness is important to emphasize. Involving ordinal space and then numbering, opens oneself to an incomputable space potentially as the first order measures are presumably cardinality on the rationals or greater, but opening up ordinality puts one in the cardinality at least on the reals. While smaller factoring can be negligible, the IQ 'full factor space' (e.g. environment, personal affect, physical health etc.) is then cardinality greater than the direct item response, so one consistently deals with that the factoring function is strictly injective even if found. This mathematically then speaks to limits by defining a set space over a space with an ordinally larger size, but highlights generally the difficulty in modeling within social theory given applicable algebraic 'collapsing' of factors. The 'field of factors' that could be effecting a particular grouping has to deal with several potential moments. Now these have reasonable solutions, but as one can analyze the basic model and determine inherently the size must be analytically reduced for any particular modality.

However as LVT makes the theoretical assumption from the 'Spearman assumption' that if one does find a particular solution this then assumed that this is an 'anti-entropic effect'. One then attributes this simplification to a compressing statement with the 'psycho-social space' however general that may be. This has been observed in IQ as being a statement on class factoring from the projection to the deviation profile, so IQ is then represented as profile shaping; 'general ability that shapes group responses' using normalized statistical curves; hence why IQ defines quotient relationships. But these then are statements on random profile and at least theoretically then cannot by a person by person theoretic order. So there is a general statement on the factor space but not bijectivity to the set response items or set individuals. Although a relationship on the set of individuals, this measure would then be better described as a class ordering than as direct set measure. This seems descriptive toward the observation that IQ factors as it has been better predictive across groups of individuals (interpersonal factoring) than individual by individuals (intrapersonal factoring). Note we have talk ourselves into existence ordinal and topological theories in this 'social space' hence why there should be a strong sense of 'openness' and 'alternate orderings'.

5.2.2 ITEM RESPONSE WITH MULTIPLE DIMENSION FACTORING

Assuming then that one has a singular factor description, one would want to refine this description particularly as first order models seem independent from ordinal factors and commutativity had limited resolution. In the example of IQ testing, there can be a multitude of factors influencing both the direct measurement (question choices, testing environment, item types) and with latent factors (individual motivation, personal differences, familiarity with testing). So a natural progression is to parse refining factors out, and increasing the cardinality on set observables then hopefully could lead to an approach that analytically refines better theoretic decompositions.

The underlying linear statistical analyses should be familiar to most statistics practitioners. However as the algebraic position poses potential problems any statistical analysis must come with simplifying assumptions, or accept a degree of incompleteness. Latent factor analysts use several modalities to categorize these split representations. Useful for this section are the concepts of measured, manifest, and latent as these are the central variable types used during refinement.

For the IQ example, measured variables would correspond to environmental factors as well as the direct test scoring. Then the manifested variables are the item responses themselves by the individuals and the hypothesized latent variables are the underlying phenomena description. So upon observation, one might notice individual test scores correspond to say that on each fifth item row there are changes in correlation between individual groups, a 'manifested phenomena'. If one can then reasonably match these 'manifested response' to say a pre-scripted 'mathematical reasoning' item set types in the measurement variables, then one can support an empirical stance that this represents some more specific latent phenomena being manifested; expression of a specific trait around question type that then maps into the latent variable space. This also works conversely; say the manifested response occurs because of question priming hence a 'measurement phenomena'. So this adds a useful algebraic simplification either way as one can assume a 'bijective section' between observations and theoretic statement (observation -> manifest -> sub-group of latent). Then with assumption infer that this corresponds to some latent sub-factoring on the more general factor, or sub-factor giving correlational space more power. If one is familiar with specific intelligences, these manifested correlational profiles are then found support for specific intelligence groupings.

As one may start to reason, finding a sufficient empirical solution for assigning manifested dimensions against supporting generalized latent factors is difficult to say the least. In the one factor case, modeling at the descriptive correlative level left with an ordering inference but limited refinement potential, and while adding measuring variables can be shown to add in statistical significance in identifying possible manifested effects, the tracing then back to the latent space which now has added dimensions is difficult. An ongoing question is then how much does one refine manifest dimensions opposed to generalized latent factors against the descriptive potential verse convergence.

Additionally useful classes help in these cases, amongst which are inclusion of endogenous and exogenous variables to describe the epistemic split between manifest and measure as endogenous and exogenous are assumed to capture manifest and generalized measure variables respectively. Here Jorgenson gives a good generalized linear structural model form that shows typical variable typing considered for analysis (Jorgenson 1978):
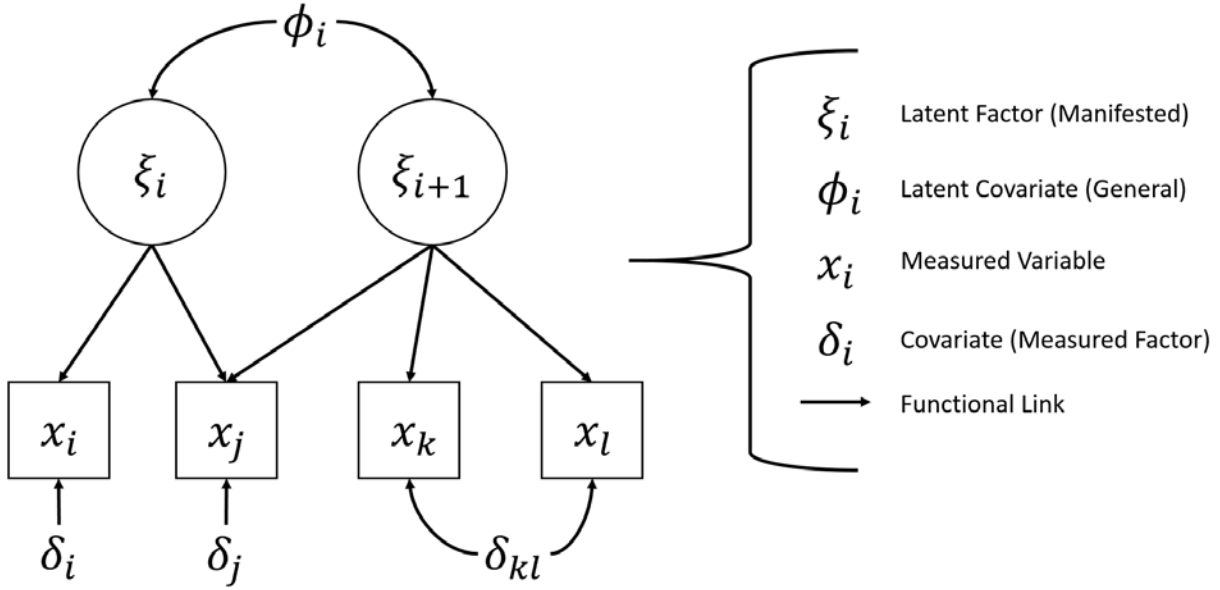
Figure 5: LISREL Graphical Model (Adapted from Jorgenson 1978)

The use on a priori typing is that this reduces the presumed analysis. If for example one has an exogenous variable, one can assume that this is not determinate from the latent phenomena within an individual. It still needs to be modeled but can serve as a basis on either a direct quotient on the measurement set or a functional description on the specific covariation factor. This then gives more granularity on the measurement space providing more precision when performing the latent factor analysis. The determination on variable typing and configuration come from experimental and epistemological consideration (e.g. psychometrics presume different use on exogenous variable compared to econometrics). However pre-typing the analysis can yield more precision within the latent space or rather more elimination on potential moments, but this involves some architecture in the design. So independence on types against orderings has to be designed and given its own alternate ordering.

With sufficient analysis and computation, various measurement observables can be used to converge to a solution, but this depends on what form the latent effect takes: is it a specific factor or is it a correlative term between specific factors? There were no universal criteria or procedures for identification. However there are common estimation tools that should be familiar. Listed below are a sampling found with typing provided by (Bartholomew et al 2002)

Let $v = (\tau, \Lambda, \phi, \theta)$ be the vector containing all model parameters

Maximum Likelihood

$$F_{ML} = \ln|\Sigma(v)| + tr\big(S\Sigma^{-1}(v)\big) - \ln|S| - p$$

Unweighted Least Squares

$$F_{ULS} = \frac{1}{2} tr(S - \Sigma(v))^2$$

Generalized Least Squares

$$F_{GLS} = \frac{1}{2} tr(I - S^{-1}\Sigma(v))^2$$

The basic estimation methodology is congruent to most exploratory analysis. Minimizing difference between fit model against the sampling, and the only addition with LVT is to include the covariate matrix and then the choice 'distance measure'. It is noted amongst review papers that for normal, probabilistic items are commonly used and maximum likelihood is then usually expected (Joreskog & Moustaki 2001). Additionally methods such as rotations and clustering are used, but given that the latent space is of importance and data manipulation directly influences these, the manipulation should either be kept to a minimum or strongly justified.

Another useful notion is using a model which is known to have a unique solution (unique matched with covariant matrix) in which case it is called 'identified'. Otherwise an exploratory model-setup is said to be 'under-identified'. The heuristic methodology is to examine what is usually an under-identified model and add constraints where justifiable until the model can be identified. As this can make for arbitrary model encapsulation, this general approach is termed Exploratory Factor Analysis (EFA); sometimes principal component analysis is used synonymously as one is 'exploring for the principal factors,' but we will define the difference in later sections. Generalized algebraic unknowns useful are on potential observable latent objects (Bollen 1989) and varieties on model parameters and degrees of freedom (Bartholomew et al 2002).

From the criteria, one can take away good guiding criteria for simple informational cases gained from psycho-social measure. There is a dualistic meta-constraint as discussed by treatment of measurable variables against the change in observable, identifiable latent space. This is just for identifying the analytic model let alone commutative against the greater state space as identified in a categorical model sense.

So then there are identifiable typing on the model viability depending on the latent analysis alone. The compression involved in estimating latent variables involves both inclusion on [measurable-manifest] observables and additions in constraint on the [manifested-latent] factors. While ideally an exploratory model fits solvability criteria and thus a bijective mapping, LVT assumes generally this is not the case, and easily identifiable behavior models seem to be exceptions rather than the case rules. There are other categorical methods for splitting this however for multi-dimensional real space these rules seem inescapable; less to say that human behavior is a complex factoring. Provided then is a functors diagram describing the measure limits described in the Rosen measure categories (Rosen 1978).
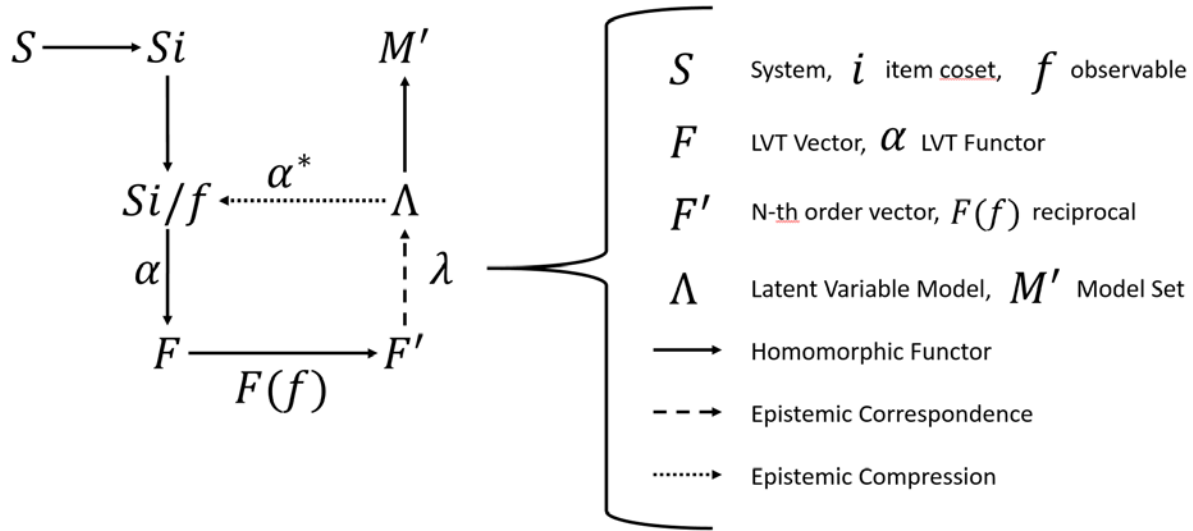
Figure 6: Latent Variable Category Diagram

5.2.3   STRUCTURAL MODELING AND CONFIRMING FACTORS

Now as noted previously, there are observable structure(s) that can be identified as this is a relatable social space. For instance, the localization of 'mathematical reasoning' would want to be tested as a hypothesis, but as one has to assume an open setting for latent structure in EFA, one can then just set these as belonging to a 'known, latent structure' (i.e. pre-scripted mathematical questions should not share factors with say linguistic questions). This provides additional constraint which allows effectively greater solvability by estimation addition. This is then termed Confirmatory Factor Analysis as one is trying to 'confirm' a particular model structure.

This becomes an inherent simplification which might seem obvious to most. But as discussed the bijectivity of humans to measure shows that constraints can be large assumptions potentially missing latent phenomena that at least as a 'warning signal' is against the purpose. LVT distinguishes between these as while EFA and CFA are even blurred in practice, it still signals a categorically different theoretic approach. More common is to use in parallel: EFA to identify negligible elements, CFA to show continued good fit, EFA again to expand to new factors, CFA to retest these hypotheses, etc. Quite synonymous with exploratory and explanatory modeling, yet as discussed, EFA and CFA can have an additional layer of theorem given the ordinal space induced by social theory.

For CFA, the starting point is a hypothesized, set model schema rather than a measurable set. The goal then is to 'confirm' this hypothesized model schema is inductively correct using analysis on 'fit statistics'. Moving to a different basis for analysis, it is then useful to categorize the schematic models as often one is trying to (un)validate a multitude of models. Here visual aids and graphical notation is often used to show the full model structure. As an interesting side note, the initial schema is often elicited from community members, and is then aligned to

model elicitation practices, so this may be an interesting overlap to systems modeling. As (Hersberger 1994) notes, the use on graphical notation can vary. However, they tend to communicate equivalent structure within LVT.

Once there is a set-model structure, a model then gains the description of being a structural equation model (SEM). This then presents a paradigm to simulate the set model, and then the goal is to gain a variety of fit statistics against a data set; or more ideally a class of data sets. As might be intuitively realized, one inherently assumes that then a model is identifiable (or semi-identifiable under probabilistic models). Then CFA's are subject to necessary (but not necessarily sufficient conditions) from Bollen (1989):

$$t \leq 0.5\, p(p + 1)$$
$$t =' number of\ estimated\ parameters', p = 'indicators$$

- Scale of Latent Variables must be set by either
  - Fixing factor variance (Ota)
  - Fixing factor loading (Lambda)

Then one obviously makes an inductive case using a variety of fit statistics to claim that a hypothetical SEM is valid. The validity and relative strength on statistics seems its own area of inquiry, and there did not seem an apparent universal criterion. However there did seem to be two major classes based either derivation of a chi-square statistic or an information theoretic basis (i.e. information criteria).

These have been implemented in various platforms
- LISREL

- Amos

- EQS

- MPlus

- GLLAMM

- Stata

- R packages: Lavaan, Psychometrics

Now here there is useful descriptive difference between PCA and CFA. In measurement environments, the full space of potential model structures and/or schemas can be immensely complex to a numerical space. However some environments are clearly more constrained than others. CFA generally is useful in this area because upon high-level analysis can help one map to assumptions based on context: a pilot in flight offers a much stronger linear basis compared to personality over food choices. More ordinally constrained environments then are more

easily fit to identifiable models, and then one rather 'monitors' that the axiomatic principals to a model are not being violated; one monitors the 'principal components' to a system against those on an identifiable model. Otherwise one is said to be 'confirming factors' in an otherwise unidentifiable system. Although just as one switches between EFA and CFA, PCA is often analogous/synonymous in practice.

The PCA paradigm seems closest to direct usage with in monitoring for 'higher order' effects. A recent example is the creation of information theoretic models for stock market behavior. The first-order model matches the units to the Brownian motion object from the measure basis (Bollerslev & Mikkelsen 1996). Then there are general theorems that present useful classes within the system explaining the possible information states that are statistically identifiable: 'long-memory', 'rough stochastic', and 'non-memoried' (Fouque et al 2000; Chronopoulou & Viens 2012). Then what financial engineers attempt is to create 'warning signals' that instead monitor that the principal assumptions within a class of model is being upheld or can reasonably be confirmed. 'Long-memory' implies there is reliable hysteresis, so monitoring just confirms that particular components are fulfilled and then allow for identifiable models (congruent to PCA). 'Rough stochastic' allows for capturable algebraic assumptions as there is a 'mean reverting' portion. But there is not enough for full identifiability, so one confirms that a particular model is viable (congruent to CFA). 'Non-memoried' (i.e. non-dependent, non-memoried) then allows for little tractable solutions, so general exploration is the only option (congruent to EFA) (Chronopoulou 2016). Then for modeling simulation purposes, one assumes that the class change maps to a representable state change in the system, and one has a reasonable if not abstract control schema. Although the algebraic rules that come with stochastic systems makes the identification of models different from traditional LVT, there is consistency in the analytic intuition, and it is our hypothesis that this due to the (latent) ordinal structuring.

While identifiable factor models are ideal, generally one has to explore variety of models as well as ordinals. There are common model assumptions that appear that are useful and considered well justified if not well identified (Moustaki et al 2015):

- Setting on latent factor loading to values

- Setting or constraining on error variances

- Interchanging error variance with correlated specific factors

- Specifying covariance on factors

- Scaling the latent variable

So the uniqueness of LVT methodology is in doing a 'two-sidedness' to the analysis as one explores modal structure and algebraic schema. Considering again the IQ item measurement, as one repeats the measure one would like to use this as a predictive simulation. However

given that there may be two (semi-)viable model schemas (those mathematically inclined vs physically inclined), then one is doing dual simulations based on the mapping on these class of individuals, and for large sets, the model being a strong compression finds specific factors within this. Or trivially, how does one split the Liar's Paradox as someone have a vendetta for any reason and may consciously miss-answer test questions.

These 'problems' abound and tend to plague most simulations of social theory, but for a particular identified model structure, one can justifiably take formal stances (i.e. claiming a philosophical stance) that allows for viable modeling efforts. (Borsboom et al 2003) have a large and extensive review here that covers the large categories on perspectives that also has references to perspectives per model type. This quickly relates to large discussions on causality, ontology, epistemology etc., so we will only pause briefly to mention that the formal stance is a philosophical one not per se one gained fully from analysis. This is important as during the review it is noticed the care that literature keeps to relating formal stance(s) towards the measured data, dimensional significance, covariate choicing, modal classes / variable typing, and modalities.

For an IQ modeling, one explores the scores for interactive factors to principal factors, and then explore the score space itself for confirming those factors against a reasonable variety of stances or previous modalities. The difficulty becomes in the dependent nature between separating phenomena within a covariate space: Is this factor in the deviation directly tied to difficulty in language between the group, specific question type, or generally a measured answer of a general factor? These become large standard moments that are difficult to place in terms of epistemology: is clustering behavior reducible to a single source and is this source attributable to a manifest or latent variable? This requires iteration to investigate the model for its nature, and iteration of measure to inductively claim that this holds across environment and individuals less it fail being 'general' intelligence. There is some reasonable art in taking formal stances, but clearly the variety contained in most psycho-social systems requires a breadth of analysis and algebraic considerations.

As PCA and CFA maintain the same algebraic description, the two analyses have consistent overlap. From an axiomatic model standpoint, there is no maintenance of a difference in numerical models as a model algebra is transposable. Consideration within mathematical psychology according to Bartholomew et al (2002) does not contend this as "in fact the two can be indistinguishable". The methods then are distinguished by 'meta-purposes' such as "intent", "hypothesis", and "experimental considerations". In fact within several reviews, the analysis program types are often "done in tandem" or "sometimes indistinguishable". Considering the IQ model, analyzing answer clustering that yield distinguishable latent fit to an identified model (EFA) often then makes good candidates for first-order factor models (CFA) often using nearly the same computational analysis.

The difference then comes under extension. When extending across groups alternate ordinals, as touched on one has to consider certain breaks in commutativity. Then PCA and CFA distinctions become important as say a PCA on individual (sub-group) scores may not

(necessarily) be congruent with a CFA model on the total group or total phenomena of interest in that group. Again for IQ, it has been found that certain PCA that yield certain specific performance groupings are not nicely congruent over a CFA program with generalized intelligence measure model (Horn & McArdle 2012). So any set factoring on an individual does not (necessarily) seem to be a reliable sub-group on the total (algebraic) grouping. This certainly opens up the perplexing areas of complexity present in social sciences as elsewhere. The uniqueness here however is in the higher order inferences that present strong considerations of method, program, and an 'algebraic intent'.

In reviewing practices in latent variable theory, it is not surprising that effective measurement programs present methodological typing and considering of experimental context. As Jorgensen notes, good exemplars often involve iteration and cross involvement on both the analysis method and other type considerations (Jorgensen Factor Analysis). Upon review there were several other sub-typings available which should not be considered exhaustive but rather exemplar ideation founded within LVT review in the next section. As there is not necessarily nice compression within measured groups across the whole, a common typing found was to consider unique mereological (i.e. group inheritance rules): considerations found were idiographic (individual ideation) against nomothetic (general ideation), class structuring, and factoring conscious processes & unconscious processes differently (Nesselroade 2012). Sub-orderings will be familiar to modelers (categorical, endogenous, exogenous), but these are still considered embedding into the same EFA, PCA, and CFA paradigms so inherit the potential 'construct validity' issues as discussed. The listing then to show a sampling of potential extensions of types that are under consideration, and as there are not clearly reducible logics due to the seeming grouping problem, modelers have to then maintain these 'meta-method types' under their activities.

Now considering the algebraic effect on these descriptions begins to get to unusual questions. As we had the functor diagram from our previous sections, left with the epistemic question of finding case refinement for particular models and system of interest. The experimental considerations then apply to a typing on the system of interest such as a considering of an idiographic nature predicates available objects different then the specific objects on a nomothetic system. This then 'compresses' the available space to a viable state space via the response factoring to an 'item'. LVT has shown that an 'item' can be abstractly extended to other behaviors given an algebraic unit to said behavior: "health behavior" -> 'visit to doctor'. With enough identification or experimental set-up, then these 'nomologies' then are thought to form a space which hopefully has enough 'identification' to form a measurable space; within which the measurable space has objects that correspond to what is ultimately 'ideas' living in the 'imaginary numerals' of a complex space. In the former, one tends to use validity on a model using 'construct validity' (if the overall construction on the phenomena is valid), and in the later one tends to use 'epistemic validity' in the similar sense that most measure theorists use. This is contingent on the seeming unidentifiability on the general space for which theory is to describe, so this presents the usage of more abstracted types to dually describe the validity on enumerated analysis and the mapping to spaces and theories with which it is to be

contained. This hopefully describes why often the classing and typing of models are more useful to generalized analysis then combinatorial methods on enumerated models.

The above discussion seems to imply a complex numeral system or even something above as the bases within the system. While there were stochastic and other methods found that touched on complex methods, material on the relation to complex analytic theorems or larger order topology were not found as of the time of this review. However, there were interesting investigations in this area including complexity (Byrne & Callaghan 2014) and even categories (Phillips & Wilson 2010). Still, this work has not yet gotten to the where these considerations can be integrated into LVT in practice.

In trying to formulate these ideas, the larger generalized information on 'constructs' still have some relations that can be observed. Even if IQ cannot be readily mapped to an enumerated explanation, across several studies one can still have a compressed description that there is some objective (if not fuzzy) relation between 'cognitive ability' and 'itemized behavioral performance' (or likewise generalizing terms). So one can observe 'fuzzy', or 'softer' theoretic descriptions that are only computable under 'identifying constraints', but the general relationship can still be accessed. Social theory cannot be too simple or else computable architectures would be more readily available.

This leads to an interesting area on the best representational means in 'communicating' these general 'nomologies' while maintaining computability or at least 'modelability' where generally observed. Cronbach, Shadish, and Trochim have interesting discussions where all suggest variation on a 'nomological network' in which to describe these observable relationships. In all there is consideration towards the generalized object groupings and their modal extensions which 'tie together' (e.g. 'intelligence' -> 'creation on specific skill' -> 'performance grouping' -> 'Item performance'). The thinking being that these 'networks' notate more general hypotheses that can make use of inductive evidence to support themselves, but then dually have competing general theories with which to form more specifying (and thus identifiable) hypotheses. These are then abstract ordinal theory that are maintained congruently across set hypotheses. This area is explored more in other sections but to show the intuition on the 'abstract encoding' that social theory entails.

Again explored more in depth in other sections, this is an equivalent description on category theoretic descriptions. Briefly a category defined mathematically is any abstract object equipped with some 'morphism' (model schema, algorithm, more abstract 'functor'), and there is growing mathematical theorems which may help provide means for specifying these 'nomologies' potential into situatable 'ontologies' by progressing the generalized space to a type set ordering. Below explored is an attempt to represent these generalizing ideas with formal functors. These have a nice morphism between them but at least upon review these only seem to happen given again particulars. PCA against CFA can gain further refined description by considering the diagram again for the model apportionment. From the point of a particular system split by observables and then their covariant space translation,
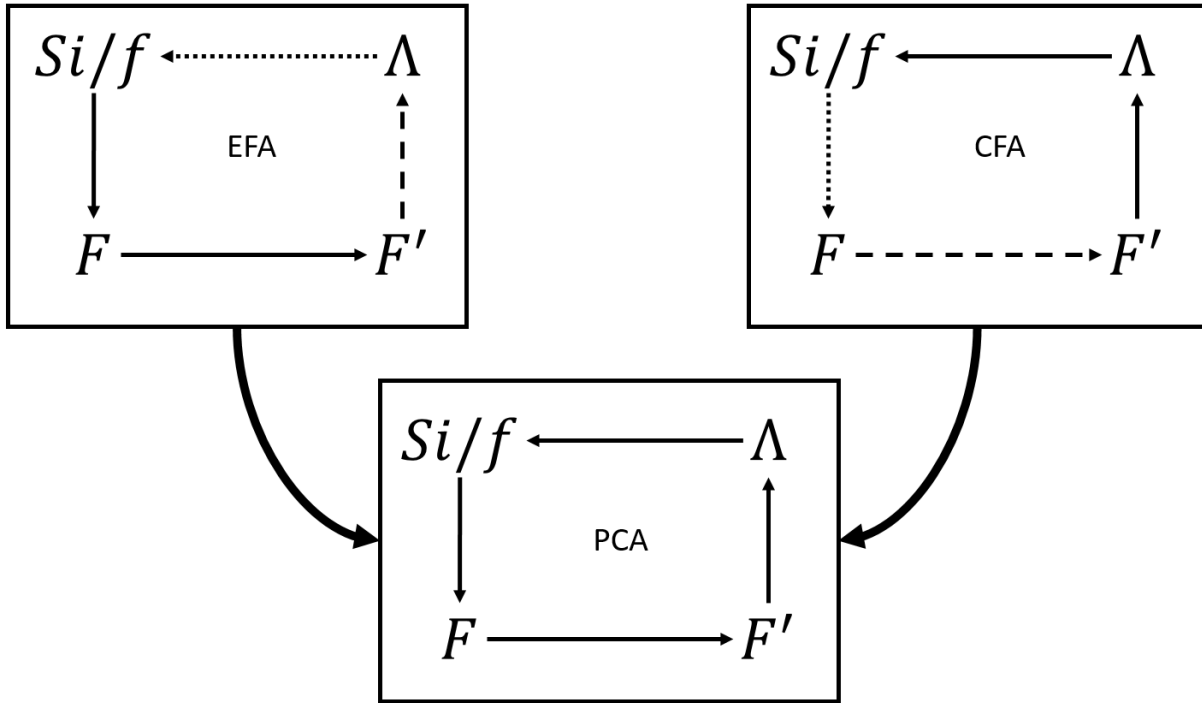
Figure 7: PCA as Colimit Adjoint

At the beginning, the starting assumption is that these are not reliably commutative on neither the covariate nor observable sub-closures. Then as one searches to find reliable objective 'descriptors' (i.e. functors) one has to consider that the left and right (co)setting are then not reliably symmetric. So one has to consider exploring into the system space from the item response (i.e. intuition upon EFA), and one has to consider mapping the system reasonably to said set item (i.e. intuition upon CFA). In cases where the system is 'identified', this seems equivalent to saying that the left and right setting are commutative and thus negligible (hence PCA being a simplifying case).

So one has to analyze 'each side' for both exploratory (defined functions varying object descriptions) and explanatory (defined objects varying descriptions), but then has to find a matching colimit as a description must be an inverting match back to the observable. In many measurement areas, this distinction can be trivial, but for a social system that can literally if not slowly inject abstractions, this triviality is not so trivial. Also as social modeling measures must explore ordinals and other structural typing, this adds the requirement to match these functions to the same invertible functors(s) in higher order spaces. If able to be set epistemically or identified, then the observable itself becomes nicely epistemically recursible.

This then can vary the theoretic algebraic grouping (i.e. object, function match) across higher orders. Both objects and functions are being searched across a bi-directional branching. As such EFA can be thought as the analytic exploration particularly on the 'left side' of the diagrammatic program, CFA as the usually algebraic exploration particularly tracing from the 'right side' of the program, and PCA a designation on exploration upon sufficiently reusable

theory. As well the variability in these object, operation pairing then presents questions not only on the 'construct' validity concerns; or whether or not a particular analytic pairing can be said to fit an available construct within the system of interest. One might find quantum theoretic objects description but then are quantum associated operations available in the system? Even if so is this quantum congruence, at the measured variant or the latent?

Definition: $(F, \mathfrak{I}_F, f^*)$ - "LVT Construct

st.
$$d(Si) \underset{...}{\Rightarrow} F'$$
$$Si/f \underset{...}{\Rightarrow} F$$
$$\Lambda \underset{...}{\Rightarrow} \mathfrak{I}_F$$

where $\mathfrak{I}_F$ - 'topology over F'
$d(Si)$ - 'distance measure'
f^* - 'recursible function'

Figure 8: Construct Definition

Then posed is the extent to which considerations become available. Even though splitting these groupings numerically becomes difficult, representing them seems a natural human ability. So one can clearly identify these as a potential encapsulated analysis and thus coded informata. While there is general treatment as noted and the base formulation is extended to other modeling paradigms, attempts to find formal theoretic information treatment was limited. For instance, one may think to use an ontology mapping for tracing typing on models, and instead find methodology in which, numerical methods become of low cost and human intuition can produce more readily changeable generalized nomological hypotheses (invoking similar patterns as 'human-on-the-loop'). As various diagrammatic formulation with varying morphic properties becomes possible, these would be couched in a natural language yet would need a settable representation for computable results.

5.2.4 MULTI-LEVELING, DATA TYPING, AND MIXTURE MODELS

In a formal manner, then PCA modeling is based in exploring linear (matrix) algebra for the latent covariate profiles. A predictive matrix algebraic equation is then explored for fit statistics. The variation and judgement is adjusted fitting different underlying model constructions along with model complexity judged against those fit statistics. So for IQ testing, choices may look against assigning scores as manifest variables or measured variables or also other sub-typings (e.g. continuous profile vs categorical) with which grouped scores again exploratory statistics along with exploring potential principle component assignment. The result then is establishing from data both a variable analysis and an analysis of abstraction structure. As for identified model structures with sufficient justification, one can embed models and make use of multivariate and multimethod simulations. This is a developing area moving towards mixture modeling and classifying identifiability and extensibility in practice. Reviewed

here will be the methodology for embedding. Also, we will present models that may be of interest to social system modeling and efforts in the systems community.

Once one has established a covariate notation, the base format can be extended across various variable types. One can represent measured ordinals variables by establishing a mapping from a latent continuous variable implying a fuzzy inference mapping to sectioned items:

$$x_i = a \overset{i}{\Leftrightarrow} t^{(i)}_{a-1} < x^*_t \Leftrightarrow t^{(i)}_{a-1} < x^*_t < t^{(i)}_a t^{(i)}_a$$
$$\left| t^{(i)}_{...} \right| = m - 1$$

$$t^{(i)}_{...} = t^{(i)}_{...} = \text{totally ordered thresholds,}$$
$$\left| t^{(i)}_{...} \right| = m = \text{"number of variable categories"}$$

Then one maps this to a latent model format by setting the measure variable to mean 1 and variance zero (as it is assumed categorical), and the factor loadings then map to threshold values. This then has identifiable solutions depending on multi-stage estimation (Muthen 1983) (Joreskog 1990,1994). With the available latent objects, there are strong examples then of translating categorical behavior to continuous space for analysis (Bartholomew et al 2002). There are then interesting behavioral examples as one can then gain models that can create predictive models which have a restricted domain (time delimited health check-ins) toward a continuous probability measure set.

Since there are successive ordinals on the model there are several choices for the model(s) although the covariate algebraic principles remain the same. Useful then is establishing the assumption to the model showing object type and variate connection to the analytic models; this is where the graphical format becomes useful to capture the assumed structure between measured variables. This then allows scripted procedural methodology by equation and profile structure: graphical combinatorial type -> model set -> method program. Then one can presume (and many have) identified categories for particular structures.

For example a 'path analysis' has a representable diagram as such below:
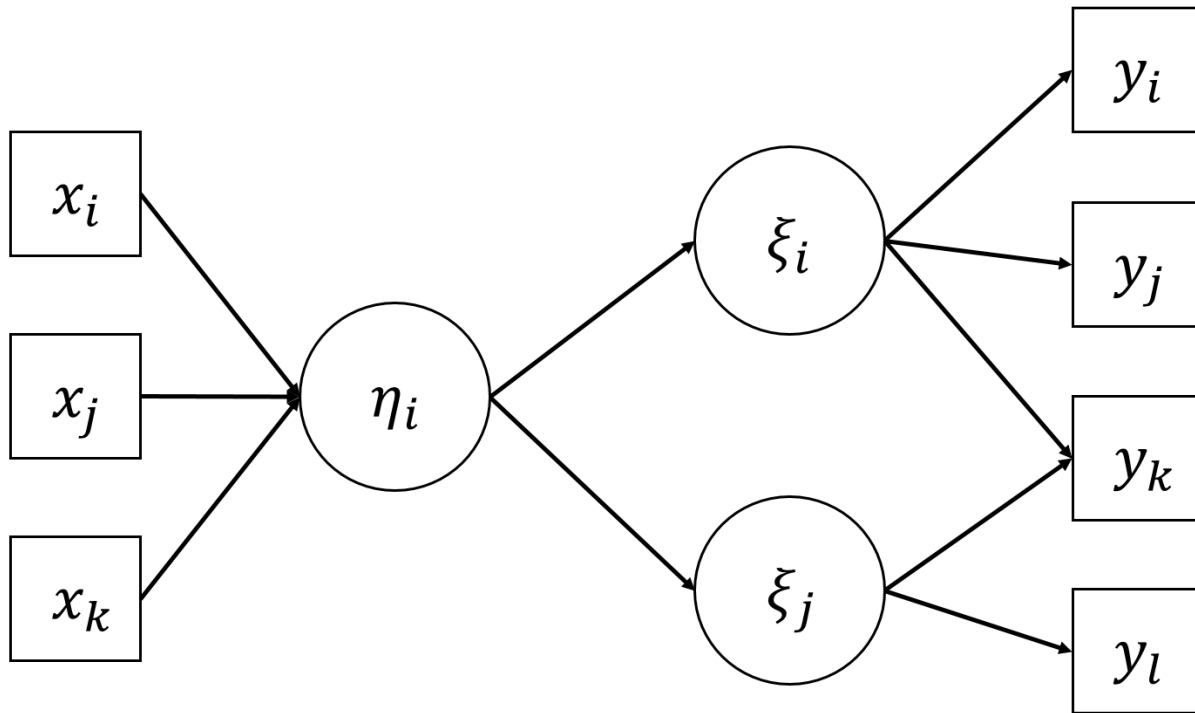
Figure 9 – Path Analysis (Adapted from Moustaki et al 2015)

One can then here estimate latent effects measured a priori that might determine latently determined posterior measurements. A clear example is a personality response that determines a behavioral profile that then shows success 'factors' that determine program outcome. This is also a common form within public health behavior in trying to find priori individual factors that across time determine measurable biological responses (Wall & Li 2009).

Generalizing the various considerations after the model set up, obvious is requiring a convergence algorithm to translate open space to a measurable space. A maximum likelihood estimate is used based on Bayesian information consideration per individual involved models. Then using multivariate covariate structures one can mix latent variables by an assumed model class assumption; e.g. linear model, growth models, etc. Then mapping these model class objects to our latent structural objects one can provide latent dimensionality to an analysis: presuming then one might search for possible ordinal responses within traditional technical analysis. This presents LVT as a means for identifying a 'space' in which a behavior might create (Wang & Wall 2003). As one hopefully notices this mimics similar structure to their likewise analytic cousin, but with LVT the purpose is to separate the 'social variant' explicitly as possible to the 'latent space' and then by extension manifested variables can be model in familiar technical ways using time series variables from ordered measured variants.

Multi-indicators and multiple causes (MIMIC) is a standard form for regression analysis using a single factored endogenous latent variable against multiple possible exogenous covariates. An example is PTSD determination (a disease potentially linked to several environmental factors)

parsed amongst a group of individuals. Useful for determining individual latent behavior against several potentially compounding inputs. A modelable example is done by (Gerwirtz et al 2010) looking at the multi-method, multi-group effects surrounding posttraumatic stress symptoms and behavior. This then leads to future a policy analysis on latent space of potential factors that helped to explain some unanticipated effects on treating PTSD against different policy groups.

Of last example, particularly related to complex system modeling are takes on multi-leveling and dynamical estimation. If one thinks to map a linear latent equation to an individual as has been shown, then one can gain a latent model mapping onto these measured determinants. Then one maps these determinants as inputs to another latent "level". A physical example is modeling person specific education model and then tracing the change in score determinants (e.g. gender, race, baselines) against change in environmental factors (e.g. classroom changes year to year). The basic intuition is to have a linear regressed model, but the slope (Individual 'Level 1') determined year to year. Then one has a latent estimate against the intercept to these regressions (Classroom 'Level 2') assessed against ordinal encapsulations (i.e. upon yearly classroom changes). Similarly growth models are estimated by mapping the latent objects to being the parameters to an identifiable system of dynamical equations. Then one estimates latent growth factors by regressing against the curve profile (Bollen & Curran 2006).

The model types become extensive as one matches a latent profile against an identifiable constraint (epistemic validity) and against the experimental description that allows theorem to reasonably map to those identifiable constraints (construct validity). That said other interesting model estimation programs are available or under research. It is useful to note here that research requires not only identifying the statistical solution, but also inductively showing this can reasonably represent a contextual class of behavior.

Below is a non-exhaustive sampling of LVT paradigms encountered:

- Multiple and Multivariate Regression

- Analysis of Variance (ANOVA)

- Multi-Group Analysis for Categorical Data (Millsap & Yun-Tein 2004)

- Latent Recursion Models

- Non-Linear Growth

- Multivariate Latent Class (Collins & Wugalter 1992)

- Autoregressive Latent Trajectory

- Indicators for Latent Exogenous Variables

- Latent Growth Curve Mixture Model

- Latent Nested Ordinal Models

Last to mention is estimation on latent classes based on these latent models. The output being a categorical informational variable that attempts to determine the class and type relation. The object mapping is then to an underlying probability space implying Bayesian network combinatorically. Then one assesses the marginal probability space using information criteria. For the extended categorical data setup, (Moustaki & Knott 2000) provides a good generalization, and (Mejlgaard & Stares 2010) shows a basic case example. Then it is thought to potentially identify an embedded ordinal model within a class (Joreskog & Moustaki 2001) which might be useful to provide estimation using Bayesian nested models.

As presented, there were useful categories given the wealth of modeling encountered. At the conceptual abstraction, multi-modeling falls back on probability and frequency assessment and thus have translated criteria to system models from information theory background. The additional criteria from the dual PCA and CFA factoring is to pay attention to the probabilistic frequency for both observed and latent variants: termed observed frequencies and expected frequencies respectively. To represent these 'predicited frequencies' there is then assumed profiles based on categorical type of the model variable. An interesting finding was the extent to which information criteria used a deviation on 'traditional' Bayesian Inference (Bayesian Inference Criteria BIC) as this prefers more parsimonious models than necessarily explain phenomena of interest. Primary alternatives were found as Akaike Information Criteria through bivariate marginal residuals (Maydeu-Olivares & Joe 2008; Reiser 2008; Bartholomew & Leung 2002) as these are thought to be more indicative of latent social variants.

After these concerns and considerations seem to get lengthy, and there is a large growing body a knowledge (Jones & Thissen 2007). Prominent terms were quantitative and qualitative considerations for epistemic and construct validity respectively. As well large scale modeling involves matching with appropriate '-ology' within the subject area: e.g. personality to psychology, group behavior with sociology. The primary agenda encountered amongst practicum groups was dually expanding the quantitative available constructs in psychometrics and econometrics particularly two areas that primarily measure agent and enterprise policies respectfully.

5.2.5   STRUCTURAL DETERMINATION & OPERATIONALIZING LVT

Here one can mention how latent factoring in social science methods begin to break more significantly from physical sciences. Physics often deals with latent factors. For example, a thermometer is influenced by latent factors such as atomic collisions, but it is sufficient to deal with the abstraction by statistically aggregating the collisions (physics latent description of heat). An even more interesting example is development of theory that explains fusion within stars. Even though physicists cannot isolate a star, examine its interior, or conduct experiments, they were able to develop a theory that explains how it works. This theory is based on a number of phenomena that are not directly observed. However, we know that this

latent model works within certain predictable bounds (e.g. temperature, pressure ranges for material state), as one can then observe measurable objective phenomena within some defined convergence space.

In a similar fashion, latent statistical criteria have bounds defined within the experimental design by the congruence between construct objects and then implied theorems (e.g. rational agent theory to econometrics). However, humans have the ability to describe their own behavior and potentially modify it. This quality makes it increasingly difficult to have an objective, (stationary) constraint about the embedded model algebras. Physics has centrally established settable theoretic descriptions (e.g. Newton's Law, Thermodynamics, and Quantum Theory) whose internal ordering is not influenced by human action; particles presumably do not possess a humanly conscious language. Even biological entities have a different abstraction necessary for their study, and human social sciences along the same extension. Social systems do have stability that one could model. However it is then understandable as modeling efforts have to actively check if the underlying construct is 'actual anymore' as the ordinal space fluctuates. This is quite complex against the model, but can be simple to a 'human system': e.g. if I am disagreeable and suddenly learn, I can actively work against the measure program by thinking consciously, critically, or even schizophrenically. This is a simple enough decision even for us to read and understand, but to a model, this would look like ordinally embedded response profiles. So 'simplicity' and ordering likely have different properties here.

Complexity within social theory then has a 'perspective problem' against a human reasoned model and where this model ordinally appears in 'real, measurable space'. This brings up an element of post-modernist theory which we wish to only mention here, but may be relevant to be aware (Susen 2015). The complex part of 'human measure of interest' is self-description and conscious language as these are the same phenomena with which we use scientific study; scientific theory is expressed in a human-readable language in the end. As many social psychology studies have found, 'priming effects' are prevalent in termed 'self-fulfilling prophecies' (Borsboom et al 2003), so these are centrally relevant to the abstractions involved that even with objectively set objects the underlying abstractions are mutually dependent to the phenomena of study. And thus independent settable objects are not (necessarily) always obtainable; or rather are attainable but then not fully objective. The short answer to this problem is consciously considering the experimental context and the construct validity issues (Shadish et al 2001). But the underlying difficulty is the injection that causes the system to change algebraic structure.

As seen previously within an established social science measure theory, these theoretic descriptions are not as easily 'insertable' or rather only under condition. Alternate representations seem to present diverging combinatoric and algebraic profiles even under the same observable quanta. These again are not absent compared to physics models, but one can observe rather the extent to which when dealing with human phenomena abstractions on objects are more complex from an algebraic perspective. Often then there are lack of symmetries at certain abstractions for system models. This begs then the question the extent to which embedding certain methods are available in the modeling process prevalent with

psych or social phenomena. Particularly as humans present conscious choice to their actions any informational modeling may be remiss in its assumed algebraic space. Hence understandably why so many are concerned with the generalized 'construct validity' along with the traditional epistemic validity. The heuristic method is to dually class and type phenomena and models combinatorically which provides for growing paradigms for modeling which should actively trouble model theory within socio-technical spaces.

However one can then ask what leverageable structure is available for modeling any 'human' phenomena at least over iteration. Within psychometrics, there is reliance on the covariate structure inherent to the response profile, but the choice on modeling is by a 'human system'. So generally a broad program is 'softer analysis' within researchers trained in psychological analysis (note not necessarily psychoanalysis as a theory) which gain general behavior classes and types. This is then crossed with available model schemata or other theory mapped to 'modellable' compressed objects. This all seems centered on the lack of 'centering' on our language and subsequent responses.

One then gets an impression on how data analysis tends to yield divergent theory in social science rather than converging theory in physical sciences as one has multi-dimensional statements collapsible into theory. For example there is theory confined to health behavior that make use of other general theory such as social-cognitive theory which captures as well as latent variable theory. However aspects then claim schema theory (compression by observed conscious schemas) and behaviorist theory both of which not thought to be 'contained' in either. This implies there is not a reasonably strict hierarchical mereology that are common in other physical science: e.g. quantum theory is thought to 'map up to' fluid dynamics upon sufficient scale even if the particular dynamics are not identified; otherwise one would have a rough 'parthood' ordering relation at least by invoked phenomena. In social theory, it is difficult to induce this mereology hence as the theoretical status on theory objects are seemingly constantly debated and many times have several philosophical stances, schools of thought, and/or contextual sub-theories.

This can then generally be transferred to any response item and then any objective results mirroring that structure as one just creates higher moments around a particular response item. From this, it is a programmatic method for assessing intended performance for intervention. This then usually has an implied n-tuples to its 'theoretical algebra' as it usually claims a particular stance or experimental context. This severally limits the extensibility and/or composability on social models as while these higher-order theories have support, but it is not well understood how these theories sans models can be reliably composed as there are several 'n-tuples' that a particular measure model 'comes from'. Due to this difficulty, there is no known tractable (or semi-tractable) program for model composition within social theory (Taylor et al 2015; Morse & Schloman 2011)!

However seemingly converse to this, there are several case examples on successful interventions even from areas involving what would be diverse theoretic areas. There are obvious successful enterprises and other social implementation profiles. Even then posteriori,

these enterprises then document these theoretic model objects within artifacts (e.g. reports, publication, models, databases etc.). An important example is the use of the rational agent in economics. The bulk of economic theory which is based on vonNeumann-Morgenstern utility, agent network theory, and economic metric theory has within a 'clearer' mereological hierarchies. Even behavioral economics seems to show that covariate profiles bias and provide more indirect influence on economic decisions. So what then one asks is the seeming theoretic disconnect!? This does seem the 'missing piece' to more generalized modeling with social or socio-technical spaces as the variety of general theory is this 'theoretic convergence problem' what social theory might term the 'nomological convergence'.

Now this is to point out the structural congruences within these LVT methods. Certainly each is concerned with different phenomena and uses models related therein, but indistinguishable is the algebraic form using covariant objects and normalized, standard moments at that. What is notable is the extent to which this provides an ongoing useful space for capturing and exploring human behavioral phenomena, and then across different first moment models; sometimes independent of choice in first order model. Not surprising is the extent to which these have been explored as 'warning signals' to 'spot' model bifurcations within other areas, and also use the same case for spotting major changes in psychology: changes in affect (Sinharay 2016; Edworth et al 2003; Nordin & Kaplan 2010), econometrics (Cho & White 2007; Blundell & Robin 2000), onset in group social state (Levy 2005; Nyborg et al 2016), and larger human-environment systems (Bauch et al 2016; Boettiger & Hastings 2013). Finding a recurrent signal amongst a covariant field is then strongly encouraged and at least within social sciences latent variable theory appears to be the growing objective standard for 'warning signals'.

The obvious problem is back mapping through social theory to identify even the general 'causal' phenomena. This may or may not be possible within an automata theoretic program, but it may be possible through injection by those possessing similar conscious language (e.g. subject matter experts); i.e. automata may not have a programmable method but paradigms such as 'human-in-the-loop' or 'human-on-the-loop' might allow it. Generally it was found that LVT was used for performance evaluation or (through its statistical cousins) general enterprise factor exploration. However, its use to inform the integration of models was not found. Hopefully, this implies future research potential.

In fact, from a mathematical standpoint, artificial intelligence and machine learning techniques leverage this by quickly exploring the covariate profile expanse across various standard moments (although they are programmed over some ontology). Although these methods are still in their relative infancy, the informational groupings around particular spaces are still used. Thus one would expect to encounter the general trade-off within automata theory: once programmed, these provide computationally cheap information calculation within halting bounds, but they are hard to assess outside a particular programmed space.

However, it at the same time raises questions gained from analyzing the algebraic structure. Discussed previously is the extent to which finding a leverageable commutative structure extends between moments, ordinal expanse, and ultimately to the measurement and the 'real

human' phenomena. Ideally, one finds at least a shifted center across the moments which then can solve the objective item from the 'root' of the 'human behavior phenomena'. This could help explain why engineering efforts to implement interoperate models has not been successful. Certainly, considering orders of moments can be tautological in causality. As velocity (a moment of position) is bidirectionally causal to position (velocity determines position and velocity is defined by position change), explaining major changes in first order model from higher moments could be considered natural occurrences within a particular model hence not a valuable causality; so what then separates uniqueness in human phenomena within open covariate sets? These would still be useful to observe (as velocity is an important measure), but the epistemic question is the extent to which a change is "a direct result from higher orders" on the functional description or "represents a significant change in model descriptions" (Scheffer et al 2009). Although to be clear, the bifurcation 'warning signals' within biological systems assume that simply identifying decoupling across a covariate moment communicates changes, but within social systems, the only available bifurcation signal generally described and theoretically tested seem to be the ordinal covariate space formulation. By Spearman's theory statement, a change in 'social natural' must be 'physically and unnatural anti-entropy', so inherently one is measuring epistemically an unattributable shifting signal within a shifting signal; not impossible but (like most human phenomena) a complex task.

Revisiting the toll road model from the previous research task (RT-138) (Pennock et al 2016), it was discussed that finding breaks in symmetric ordering did not have a sufficient solution without the known ordering method. One of the reasons is that individuals respond to new signals, but the change in order on the behavior left us with a non-linear attribution. Certainly using a marginal price model makes intuitive sense on one hand, there are then control questions on the other. A priori one would like this ordinal 'functor' (what are people actually thinking) rather than the specific ordering (how are they acting). The former allows a priori control and configuration and the latter might totally disorder the schema as individuals were choosing the more expensive lane. The choice to the engineers and decision makers is that one involves a configuration change and the other upends the entire set toll system.

Then one considers the algebraic observations as discussed. For a particular 'latent signal' measure, one normalizes and/or centers around a particular (algebraic) grouping behavior. This is the basis for the covariate moments which then creates the available field(s). As can be seen with examples, identifying the location of these commutative groupings (and evaluating then their validity) is the hardest part within these methods and seemingly where the art is. As examples within psychology phenomena (e.g. behavioral economics and social psychology), the basis structure that underlies standard models contain both self-referent and bias effects amongst others. This can directly effect the algebraic structure at least considered from the formal model perspective. For example, a well-known Keynesian macroeconomic description is his suggestion that people in markets might center around different measures in terms of behavior but could also consider centering around others behavior (his famous 'beauty contest' example). We could say more abstractly, without necessarily taking his direct claim, that 'people' actively change the structure of their behavior in some form or else innovation and creativity would not be human traits. Even then, broader topological and complex claims

further complicate the potential structure (Casti 1982; Kauffman & Johnsen 1991; Dixon et al 2010; Wolpert et al 2012).

This creates an underlying difficulty in relying solely on unitary, formalized system description. Singular 'warning signals' measure systems were not able to be found that did not have some difficulty with above discussed limitations. These 'systemic methods' and 'structural investigation' were common research topic areas amongst social science areas. However, what was noticed is the extent to which researchers and practitioners use the methods, but use more abstract reasoning across algebraic classes mentioned above. For instance the previous example of financial systems where there has been interesting work in finding classes in trading behavior. The bases are considerations on Brownian objects, but while the formal models are not universally reliable fits to constructs, one can use the model and its extension to reason about when a market might move through 'types'. This is not universal in its next step, but provided a 'signal' to people familiar with what a type might entail. The example classes ('long-memory', 'rough stochastic', 'non-memoried') corresponded to major changes in formal model structure respecting the traditional Brownian and Bayesian assumptions. For example, if one can class say depression screening in health behavior, knowing when a group suddenly changes profile is a strong impetus for greater attention within an administering enterprise even if one cannot gain individual by individual signaling. Additionally one could have a 'dual signal' that are orthogonal with MIMIC for individuals and multi-level for program screening which could help refine potential sub-groups yielding several of these 'signals'. This is unlikely to be reasonable in an automata way but easily 'pre-identified' based on the context by conscious modelers and interventionists. Upon softer analysis, most intervention literature seems to share this intuition while implementing LVT methods iterating on EFA and CFA profiles using various types of data.

While each model had varying computational potentials, more of interest was the analytic properties that could be assessed from each model class. For example 'long-memory' provides more informational derivation and thus solvability for determining underlying latent effects. In information theory terms, given a certain model class, the underlying 'channel space' is determinable under a certain available algebraic structure, or it has a diminished structure which then is determined by choice on model paradigm. Conversely there is reason that a sufficiency over a 'signal' would shift under a new algebraic system. This can imply both the gain in 'signal' and gain in analytic and computation aspects; e.g. sample size profiles, presumed data schema types, computation complexity needs. This then makes available potential trade-offs however broad or abstract that could drive economic or decision theory considerations which could help guide enterprise system architecture.

Additionally within discussions of the models and given by the construct question, there are additional questions toward which model classes are available 'in the real world'. How do both variables and extensions on a model provide a congruent description for the system of interest (i.e. structured behavior while trading)? This is a challenging problem as this implies considerations of meaning, behavior, structure, and ontology which are difficult issues in social theory. While we explore potential solution using the idea of nomological network across

category theory in Section 7.2, it should be explicitly stated that this is the crux of the challenge of developing more generalized methods.

5.2.6 CONCEPTUAL THEORY DISCUSSION

Through the review of latent variable theory, there are several conceptual points that can be observed toward the purposes within systems engineering as we have alluded toward. The most direct being the formal methodologic approach to data and models involving any human behavioral phenomena. More removed are both the opportunities or rather observed complications if one attempts to create a formal system from social modeling. And from a general systems perspective, the notion of construct validity and similar theoretic considerations naturally bring up notions to insert into epistemology and interoperability. One first-consequence observation one can make is that the LVT procedure fits a category theoretic encapsulation or rather a powerful enough language for its theory. The category objects being the variant spaces (plus or minus embeddings in the case of nested models), and the morphisms are either the projections of these spaces into 'identified space' or the computational solving when able to be 'identified'. Respectfully, the observational variables, their moments however defined, and then the choice eigenvalue cosetting within the latent variable(s) are definable algebraic objects then typed within a 'construct paradigm' (e.g. LISREL or Multi-variate models implied by available objects with an experimental set-up). Each has a choice on model structure within a defined measurement (categorical) object, so are then presumably settable within a context.

Now the categories as we discussed have larger extensions in pure mathematics, but use here provides a mathematically reasoned way to compare technical elements (e.g. statistics, computation) against 'psycho-social' ones (e.g. 'intelligence', 'personality', 'behavior'). Particularly as the 'construct validity', using Spearman's intuition, the goal then may be to identify first-order models that capture as best as possible naturally described elements, and then the remaining covariate space can then be reasoned to hold behavioral phenomena within its 'lens'. This or else the covariate measure becomes a 'bicategory' which requires some a priori knowledge of the structure; possibly why areas such as economics have more 'granularity' on their behavior as there are more classifiable theorems but why then behavioral economics seems more complicated given the prevalence of behavioral considerations.

For systems engineering purposes, this 'dual space' seems to be recognized by many either within areas of intervention science (Strauss & Smith 2009) or enterprise systems research (Pennock & Rouse 2015). This then begs a line of questioning on whether are not there are categorical information potentials here; from (Strauss & Smith 2009) other references with which focus under systems engineering are erdogic-ness (Borsboom et al 2004), measure abstraction (Messick 1995), informational (Kane 2006) and categorical (Clark 2006) incompleteness, and relative validation (Cronbach 1988). This is not surprising given from Thurstone's take as being a practiced engineer, the creation on statistical (i.e. 'technical') measures was for basing the behavioral measurements, and realized himself the "[injected] subjectivity toward choicing an objective statistical program" with which others can respond in

variety (e.g. correlation-causation, priming, self-ordering etc.). IQ, although well researched and practiced, now still has a centralized tautology on measuring that the quotient relationship still has set representation, so our intuition may be that this still shows some normative subjectivity (although at some point an Occam's razor argument becomes valid). So the begged question is not per se how to choice the optimal measure or computation, but rather which one 'focuses' the measure such that tangible dynamics are mapped discriminately between objects and psycho social dynamics; what researchers seem to mean when discussing 'does the measure capture the correct construct'. This then implies a 'topological approach' (e.g. Dedekind cuts) as in LVT one maps manifested (i.e. tangible items) to numerical space and uses the open real space to given latent objects measure.

The possibility on providing categorical theoretic encapsulation is that this provides system engineers the possibility to have reliable theory with which to pattern the 'socio-technical' (or theory where possible). If one has an architecture such that human behavior can be mapped as discussed in the previous paragraph, there can then be expected signaling from human or social elements. Presumably then one can pre-analyze a particular pattern that maps to an identifiable LVT model, and have then some measure on what needs classification (e.g. data types, LVT structure, model combinatorics). This as we discussed is then an identification on the kernels that the LVT information is based: mapping on the topological space, and the measure-computational limits implied. As well as LVT as provided combinatorial diagrammatic maps, these LVT models can have pre-set categories. Given this basic category, it has been shown that these category types can be mapped to a database schema (Spivak & Kent 2012), so then LVT can presumably have some automata on them for their analysis; at very least given programming on the choice eigenvalue setting. Also given by Spivak is that once a category is sufficiently defined within the category on sets it has mapping directly to a relational database schema, so potentially could help with experimental design to provided more agile experimental schemata something that limits current social measure in practice (Moustaki et al 2015). This could also potentially define where more sophisticated measure such as machine learning could be classed similar to complexity theory in terms of their inference potential.

From the schema outside the computational programs, this also gives general patterning with the engineering design and architecture itself as mentioned. Many areas within enterprise science and intervention science often use 'soft analysis' or 'open architecture' methods. The categorical mappings could be used either to more effectively 'translate' these expert formulations into procedural practice (or rather map to where openness appears in practice) and where LVT or similar methods could help validate these models. Since these measures deal with selective moments and strong ordinal complexity, pre-defining much of the architecture will be difficult, so then one would want continual monitoring or KPIs as needed where these 'open spaces' lie, again where LVT statistics can assist. Then ideally one would like to pre-identify where these KPIs should be scripted and an objective as possible framework for update and response and would then need to at least identify a general social pattern which could then have a knowledge body on similar constructions.

From this, it is our conjecture that these are notions on abstract structures which are assumed to be induced in LVT. Then these underlying construct questions become more notable when formulated in categorical theoretic terms; either by expanding a base category or decomposing property over a generalized functional class. The underlying questions raised by performing engineering activities on phenomena that are human at some component level then inherits a dialectic; while human behavior is clearly describable by formal systems, the human being consciousness in this system induces choice which to the system will be seen as state-linkage or worse at a categorical level by higher ordinals. Then having knowledge of the limits on numerical and information systems by Gödel and Chaitin respectively, one faces an 'incompleteness limit' that defining properties exist outside an embedding on the formal system itself. This problem is covered in so called 'doxic paradoxes' (i.e. 'liar-like paradoxes') and similar constructions over behavior against even a defined area such as game theory (Koons 1992; Simmons 1993).

So it is then given these 'unconstructed' sets, one expects that it is impossible within bounded rationale and resources within the formal system itself to have a program. But people in enterprises can describe this openness or incompleteness reasonably well if not poorer at 'knowing' exactly what it is; identify the areas for openness for example within '-ilities'. However then one deals with subjectivity, relativity, or similar paradox that exists within these 'natural human logics'. Now one can delve into post-modernist ontologies, but telling within research is the extent to which these behaviors are considered within the fields. But this can lead to heuristical theory and observation, so will need some underpinning if nothing else for tractability. So ideally one may like to have a space to identify past behavior, a space to translate consciously identifiable elements (i.e. LVT), or at least have a measurement paradigm to update based on linguistic information. But note these require some objective language with which to guide practice.

Taking a general approach necessary for a systems engineering, the difficulty is not then in its representation per se as one can easily have an individual model or a group model. But rather than in the logical programs when attempting to simulate or apply these together theoretically. As Borsboom et al (2003) note in an example,

> *"the [factor model] in research are between subjects, but if a within-subjects time series analysis would be performed on each of these subjects, we could get a different model for each subject. In fact Molenaar et al, have performed simulations in which they had different models for each individual (pair wise one-factor, two-fact model, etc. for each individual). It turned out that when a between-subjects model was fitted to between-subjects data at any specific time point, a factor model with low dimensionality provided an excellent fit to the data, even if the majority of subjects had a different latent structure. ... Thus, the mechanism at the level of the individual are not captured, not implied, and not tested by between-subjects analyses without heavy theoretical background assumptions that are not simply available. ... And this implies that the causal statement drawn*

from such a measurement model retains the [original assumed structural form]. (Molenaar et al 2008)"

This is an uncertain notion that not only are psychological measures latent as most scientific logical programs assume, but that latency within certain spaces may or may not have any definable linkage within the measure space (i.e. no 'identified' 'field extension'). This would appear that group phenomena has a linear independency from those in the individual, but at the same time, physically the individuals are a basis for the group ('group' does not exist without individuals)!? Realistically one can appreciate why this happens, but this creates underlying problems when defining mapping to a vector from these models.

Even then social sciences often deal with then measurements that are at the same time potentially theory irrelevant; what have been termed 'construct irrelevance'. So even one could think to constructs being locally irrelevant within a defined LVT model; e.g. presumably behavior like 'ticks' or un-conscious behavior depend little on an individual's attention. It should then not surprise that several have noted that any system with a social human becomes complex. This can be seen in an example model on Uber driver behavior as behavior can be seen to go 'in and out' of the assumed 'rational agent' model upon different criteria (Sheldon 2015). Again one reasons on what underlies these transitions, but it is difficult to prescribe to a particular model when the underlying phenomena presents a null set to that 'construct'. Rather one ordinally notes what variables excite one model construction or the other. These then become difficult to know a priori and again makes composition considerations difficult, and this invariably increases the order of the model.

The implications to this will be addressed in other sections, yet the purpose here is to establish awareness on these underlying categorical changes to programs within the social sciences. Thus we use this to support our conjecture that categorical logical rules will need to incorporate these 'changes in abstraction' necessary toward any programmatic method. One can also then touch on why there are arguable replicable patterns in social psychology. But with the given difficulties, it should not surprise that objective replicability is currently suffering in the area (Schooler 2014). Similarly, this leads to the larger scientific program within social theory as one needs to investigate over categorical abstractions; hence why there are common dualisms and dialectics in social theory; behaviorism vs. Gestaltian psychology, political economic 'schools of thoughts', and 'rational agent' & 'behavioral agent' models in economics. Just as quantum theory developed a quantum logic, social science has their own uniqueness that requires a logical system and that where axioms on 'social science' might be better represented or need to be regularly exchanged.

Given that the logical breaks happen in an 'abstract algebraic space' then categorical theory is a prime candidate as Peter Smith notes "category theory gives us a way of dealing with these layers of increasing abstraction. So if modern mathematics already abstracts, category theory comes into its own when one abstracts again and then again" (Smith 2016) (also recommended is Awodey 2010). Also of initial interest is those practitioners who note the use on patterning,

approximate, and agile orderings given its use over algebraic topology (here Cordier & Porter (2008) is a good treatise formed in categories). If we are to map (and thus get an effective statistical signal), the dialects within the social theory must be mapped across abstract spaces to obtain objects and functors in which identify means to analyze these within formal systems. Ideally one hopes to do this in a reasoned manner which means one must have a logic in which to do so in an objective manner. As of current research, category theory is the only known a priori logic that describes the abstractions herein with appropriate power.

While topological considerations in social science were encountered (Kluver & Schmidt 1999), it should be noted that abstract algebraic considerations were not sufficiently found outside of those necessary for a particular analytic program. Although the abstract considerations seem to these researchers as algebraic in theory, the notions are not currently formulated in abstract algebraic terms even against the 'non-finitist' schools. However there are relevant considerations on category theory that have shown increased attention within engineering and particularly in computer sciences. These are explored in other sections, but to mention the potential in interoperability between these abstract social modeling and system engineering methods should be strongly theoretically supportable given future research. Given the increasingly common language, this presents an opportunity for merging the 'social' and 'technical' theory embedded in these systems.

5.3   IMPLICATIONS FOR FINDING COUNTER-INTUITIVE POLICY IMPACTS

While the physical sciences and the social sciences take very different approaches to dealing with multiple ontologies and identifying unexpected consequences, at an abstract level, the fundamental problem is the same. A counter-intuitive or unexpected result, is by definition a mismatch. This mismatch can occur when comparing models to each other or comparing models to data. When we call a result counter-intuitive, it is often because the prediction of the mathematical or computational model or does not match the prediction of a human's mental model. When we call a result unexpected, it is often because the prediction of the model does not match empirical data. In both cases there is an issue with missing information.

If we view a model as compressed data and the model is incorrect, that means that either critical data was missing at the time of compression or that data was discarded in order to achieve the compression. Thus, if we have an unexpected consequence of any sort, it means that we are missing information in our model. If we want to predict the consequence with our model, that information must be put into the model somehow. In the end, there are only two sources for this information, empirical data or theory, and theory is also compressed data.

When we consider the physical sciences, there are well validated theories that seem to perform well in isolation within certain bounds. However, when those bounds are crossed, there may be no obvious way to this. So modelers attempt to connect the existing theories by using empirical data to introduce the missing information. The problem is that the validity of the existing theories does not automatically transfer to the composite model. Thus, the composed model, is

in a sense, a new theory, and the "tuning" process on establish a localized validity. Consequently, it is difficult to have confidence in projections outside of range of evaluation.

For the social sciences, on the other hand, it is difficult to even establish a reliable compression of the available data. So much relevant data is dropped during the compression process, that it is difficult to develop stable models at all. Consequently, there is often a proliferation of alternative theories and even ontologies in the social science. However, this is informative in its own right. Each of these alternative theories could be viewed as generators of potential unintended consequences that have some validity. We know that each of the established theories was correct at least often enough that it became accepted. Thus, comparisons among these alternative models are potential sources of unintended consequences.

If we are concerned about counter-intuitive policy impacts or unintended consequences of a policy, this suggests that any experienced "unintended consequences" were the result of information that was omitted from analysis. Sometimes we informally call these higher order effects. But from the perspective of this analysis, the consequence may have been predictable had the proper information been injected. Empirical data would be preferred, but this is often impractical for many policy analyses. Consequently, the only other source is theory. Yet, as we have discussed, for behavioral and social issues, there often many possible alternative theories. But which one is the right one? As the previous section found, we usually do not know a priori. Thus, are only option is try to multiple different model configuration and generate a spread of scenarios. Beyond empirical data, this is the only way to "catch" an unintended consequence or a counter-intuitive result.

This leads us to the conclusion that to have a viable approach to detect unintended consequences, we must have a systematic way to introduce alternative structure into a model. In the case of the core-peripheral approach, the core is effectively the first order model that links the decision variables to the output variables of interest. The peripheral models are alternative "theories" for how portions of the enterprise might behave. Thus, we need a way to systematically explore the space of possible peripheral models and then integrate them with the core. This creates two technical challenges. First, the core and various peripheral models may have very different ontologies. Even worse, these may overlap, meaning that they attempt to represent the same "thing" in more than one way. To overcome this, one needs a mathematical understanding of the rules that govern when and how models with multi-scale ontologies may be integrated. This will be addressed in the next section.

Second, the space of potential model permutations is vast. Since it will not be possible (or even necessary) to try them all, what is an appropriate way navigate through this space without an obvious dimension to order the models on? This will be discussed in Section 7

6   MATHEMATICAL ANALYSIS OF MULTI-SCALE ONTOLOGIES

As discussed in Section 5.1, multi-scale and multi-level models have become popular in the physical sciences and engineering. Implicit in these approaches is that the models are actually composable, yet it is well known that the composition of heterogeneous models is a non-trivial endeavor (Taylor et al 2015). Mathematical definitions of simulation interoperability and composability have already been developed (Weisel et al 2003). Rather, the interest here is understanding what leads to the interoperability and composition issues in the first place. The Levels of Conceptual Interoperability Model (LCIM) indicates that a lack of conceptual interoperability among models with regard to the reference system can cause such issues (Tolk & Muguira 2003, Wang et al 2009). The objective of this section is to develop a mathematically rigorous explanation of what it means to have a lack of conceptual interoperability among models as a consequence of the characteristics of the system being modeled and the selected abstractions. The intent is to provide a first step to understanding and facilitating the composition of models and simulations to support the development of multi-level models of enterprise systems.

To accomplish this, Rosen's (1978) approach to measuring and analyzing systems using commutative diagrams over sets is adapted. This approach provides a mechanism with which to explore the underlying linkage relationships among diverse systems views. The nature of these linkage relationships impact the ability to compose the associated models.

To that end, three categories of linkage relationships are introduced: unlinked, state linked, and transition linked. Examination of the multiscale physics modeling literature provides insights as to how these categories are addressed in practice. The outcomes of this analysis are a definition of conceptual interoperability as a lack of transition linkages across models and a set of four hypothesized sources of transition linkages among composed models.

6.1 COMPOSITE MODELS IN ENGINEERING

Models have long been used to support engineering decision making. However, one of the recurring themes of systems engineering is that multiple perspectives and hence multiple models are necessary to understand a real world system. This viewpoint is evident in architecture frameworks such as Zachman (1987) and DoDAF as well as markup languages such as SysML and IDEF that explicitly facilitate the conceptual linkage among diverse system views. The logical consequence is that to support *systems* engineering decision making, one needs to compose models from multiple perspectives. The formalization of this principle is known as Model Based Systems Engineering. Dickerson and Mavris (2013) provide a detailed history of the evolution of MBSE and the formal mathematical foundations of system design.

While such approaches allow for the computational exploration of trade spaces by propagating high-level changes down to the physics-based level, it is also necessary to propagate low-level impacts back up. While the latter can be accomplished through empirical testing, that can be an

expensive and time consuming approach. Unfortunately, accomplishing this computationally has been challenging to do in a comprehensive way.

The rapid increase in available computational power over the last several decades combined with growing inventories of computational engineering models and simulations have led many to wonder if we could accomplish the ideal of a comprehensive tradespace exploration upfront by computationally connecting existing or adapted models. In principle, this composition achieves two benefits: First, it would allow for the computational exploration of trade spaces by propagating high-level changes down to the physics-based level and propagate low-level impacts back up. Second, it would facilitate tracing impacts across diverse system viewpoints such as the cost view, functional view, etc. Some have termed the comprehensive use of integrated engineering models throughout the system life-cycle Model Centric Engineering (MCE). Regardless of the name, a successful composition of independent models is required.

The idea of computationally composing existing engineering models from multiple perspectives to assess system designs is not new. One example is Multi-Disciplinary Optimization (MDO) in aerospace engineering (Yao et al 2011). There have also been a number of attempts to develop general model composition frameworks in recent years. We will briefly mention three. First, the most well-known is the IEEE standard High Level Architecture (HLA) (IEEE 1516) (IEEE 2010). HLA provides a generic framework for federating multiple simulations via coordinated execution and data exchange. Second, SPLASH is a framework developed by IBM Research for loosely coupling models from different domains using a description language called SADL (Barberis et al 2012). Third, the Dynamic Multilevel Modeling Framework (DMMF) was an effort by the US Department of Defense to compose existing simulations across four levels: campaign, mission, engagement, and engineering to support system design and acquisition though it was ultimately dropped due to infeasibility (Mullen 2013).

As far as actually integrating composite models into the system engineering process, two efforts bear mentioning. First, OpenMETA is an integrated tool suite that was developed as part of the DARPA Adaptive Vehicle Make program (Sztipanovits et al 2014; Sztipanovits et al 2015). It allows one to reuse and compose existing engineering tools to design cyber-physical systems. The objective is to achieve a "correct by construction" design and avoid late redesign. Second NASA's Jet Propulsion Lab has an Integrated Model-Centric Engineering (IMCE) initiative that aims to better integrate engineering models across multiple disciplines into the systems engineering process for its space science missions (Bayer et al 2011). Anticipated benefits include increased reuse of existing engineering solutions, continuous verification and validation, and more rapid exploration of the design tradespace.

Friedman and Leondes (1969a,b,c) recognized the challenges of assessing internal consistency across multiple system models and developed constraint theory to do so. More recently, the National Science Foundation held a workshop to identify research challenges to using modeling and simulation to engineer complex systems. As the workshop report notes, "The reuse of models is confounded, however, by the fact that they are peculiarly fragile in a certain sense – they are typically context-sensitive, highly purposeful abstractions and simplifications of a

perception of a reality that has been shaped under a possibly unknown set of physical, legal, cognitive and other kinds of constraints by a modeler, or modeling team; quite often a model's function is sensitive to many unstated assumptions. The end result is that model reuse can be fraught with significantly more complexity than, say, reusing the implementation of a sorting routine." (Fujimoto 2016)

Consistent with the above observation, frameworks have also been developed for domain specific composition of simulations. A recent example in the area of infrastructure modeling is provided by Grogan and de Weck (2015). Another in the area of modeling logistics systems is provided by Sprock and McGinnis (2014).

Several questions naturally follow:
- Why does the computational composition of engineering models work well in some circumstances but not others?

- Why does being domain focused seem to improve the chances of success?

- Are there any indicators that would let one know when composition is feasible to attempt?

- Are there standards or approaches to model design that would facilitate future composition?

These questions have certainly been asked before. Those who have experience building composite engineering simulations probably have intuitive answers for them. The objective of this analysis is to develop a mathematical description to make certain aspects of that intuition precise. In particular, we wish to consider how conceptual interoperability or lack thereof among heterogeneous system models affects the composability of said models. The intent of the mathematical description is to serve as a mechanism to frame hypotheses regarding the above questions.

6.2 APPROACH

Developing a mathematical description of the role of conceptually interoperability in model composition is tantamount to modeling modeling. While there is an entire branch of mathematics called model theory, it is concerned with the concept of modeling in general. However, here we are concerned with some very specific questions:
- What does it mean mathematically to model a system from multiple perspectives?

- What conditions does a successful composition of multiple heterogeneous models imply with regard to the models and the system of interest?

- What attributes of the models or the system of interest would cause a composition to fail?

- How have those causes been addressed in the past if at all?

- What are the implications for MBSE and MCE?

- How might the resulting challenges be mitigated?

Consequently, the author chose to adapt Rosen's approach to modeling systems as developed in the monograph "Fundamentals of Measurement and Representation of Natural Systems" (Rosen 1978). Rosen's concern was how to measure and model natural systems and the associated implications for physics and biology. More specifically, he was interested in the interrelationships among different perspectives of a system. Thus, Rosen's work provides an appropriate set of mathematical building blocks to explore the above questions.

The investigative approach taken is as follows:
- Adapt Rosen's work to describe mathematically what it means to model a system from multiple perspectives

- Extend that description to define the conditions for the successful composition of multiple models

- Analyze the description to identify potential deviations from these conditions

- Analyze the description to see how the deviations might be addressed

- Compare the results to findings from multi-scale physics modeling

- Draw inferences about the implications for engineering modeling

- Define hypotheses and research questions for future investigation

6.3   A MATHEMATICAL EXPLANATION OF MODELING A SYSTEM FROM DIFFERENT PERSPECTIVES

The goal of this section is to express very precisely what it means to model a system from different perspectives. This is accomplished by adapting the work of Rosen (1978). Rosen used a combination of equivalence relations and commutative diagrams over sets to explore relationships among multiple views of a system[13]. We consider the following topics in sequence:
- What does it mean to view a system from different perspectives?

---

[13] The ideas presented in this subsection are attributable to Robert Rosen. However, Rosen's original presentation is very abstract with few explanatory examples. The researcher's contribution is a tailored summary and explanation of those ideas in the context of engineering modeling. The author attempted to maintain as much consistency as possible with Rosen's notation in order to facilitate comparison with his work. However, some departures from his notation were unavoidable due to differences in focus.

- What are the relationships among these perspectives?

- How do we model a system from a given perspective?

- What are the relationships among models of different perspectives?

To facilitate the discussion, we will introduce a very simple example from basic physics and revisit it throughout. Imagine a simple, one-dimensional universe that contains only two massive bodies whose attraction is governed by Newton's law of gravity $F = Gm_1m_2/r^2$. As the different components of Rosen's framework are introduced, we will consider what they mean in terms of this example.

6.3.1 WHAT DOES IT MEAN TO VIEW A SYSTEM FROM DIFFERENT PERSPECTIVES?

Rosen starts with the assumption that a system is defined by a set of states, *S*. How do we know what elements make up *S*? According to Rosen, we do not know. The best we can do is measure observables and make inferences about *S*. In terms of our simple example with two bodies, observables would include their positions, temperatures, masses, and so on. Mathematically, observables are functions that map the state space, *S*, to another set such as the real numbers.

A given observable, *f*, generates an equivalence relation R_f on *S*. That means that any two states $s, s' \in S$ belong to the same equivalence class if $(s) = f(s')$. As a result, we will be unable to discern differences in state that occur within the same equivalence class using only the observable *f*. For example, if we only measure the positions of our two bodies, we are not able to differentiate among system states that have the same positions but different temperatures.

Of course, we can measure more than one observable. A set of observables, *F*, generates an equivalence relation, R_F, on *S*. For example, if *F* consists of both position and temperature, under R_F all states of *S* that have the same temperatures and positions would be viewed as equivalent. The quotient set S/R_F is the reduced set of system states that result from the set of observables, *F*. It is a partition of the set *S*. For our simple example, we have reduced the set of states to a set of vectors of positions and temperatures.

It is important to note that the reduced state space of the system, S/R_F, is a consequence of which observables are collected. Thus, each set of observables constitutes an abstraction of the system. This provides a precise way to express what is meant by viewing a system from a particular perspective. A perspective is the quotient set generated by the collection of observables applied to a system.

Beyond understanding the current state of the system, it is also of interest to understand how the system changes states over time. The chosen collection of observables also affects what

state transitions we can discriminate. Rosen defined changes in the state of the system as an automorphism on *S*.

Let *T* be an automorphism on *S*. If *T* is compatible with R_F, then *T* induces an automorphism on the reduced set of states , S/R_F. Let us call this automorphism T_F. This is a description of the state transitions for reduced set of states S/R_F. Introducing the composition operator generates a group of automorphisms from T_F that can be used to define trajectories in the reduced state space. Indexing the resulting elements of the group by $t \in \mathbb{Z}$ or $t \in \mathbb{R}$ describes changes in system state versus time. For our two body example, repeated applications of T_F would describe how the positions of the two bodies change over time. We call this the system's dynamics.

How can we determine T_F? Again, we cannot do this directly. We can only infer it. To complicate things further, observables are not measured directly. Rather, specially configured systems called meters are used. Meters are designed to dynamically interact with the system of interest and asymptotically approach a value taken to be the measurement of the observable. An example would be using a thermometer to measure temperature.

Assume that M_F is the meter that measures the set of observables *F*. To understand T_F, we take successive measurements using the meter M_F and try to infer T_F. This situation is expressed by Equation 1.

$$
\begin{array}{ccc}
S/R_F & \xrightarrow{\;T_F\;} & S/R_F \\
\downarrow & & \downarrow \\
M_F & & M_F
\end{array}
$$

Equation 1

This setup allows us to express the impact of an abstraction defined by a collection of observables *F* on the perceived dynamics of the system. If, *T* is compatible with S/R_F then T_F is a bijection and the dynamics is deterministic and reversible. However, since S/R_F reduces the set of states, there is no guarantee that elements of *T* will be compatible with S/R_F. For many realistic problems, it will not be. The result is that T_F will split equivalence classes of R_F. This situation enables us to discriminate among more states of *S* then we could with *F* alone, but it also makes the system appear stochastic and/or irreversible. Since, we often encounter such situations in real life, we will only require T_F to be an endomorphism as opposed to an automorphism for the remainder of this paper.

6.3.2 WHAT ARE THE RELATIONSHIPS AMONG MULTIPLE PERSPECTIVES OF A SYSTEM?

Extending the idea that an abstraction of a system is determined by a collection of observables, we ask how we can precisely define relationships among multiple abstractions of the same system. These relationships are known as linkages and they can be defined by which combinations of equivalence classes from each of the perspectives are allowable.

Assume that a system can be described by two observables $f(s)$ and $g(s)$. Each generates an equivalence relation, R_f and R_g respectively. If both are applied at the same time, the result is the equivalence relation, R_{fg}. What is the relationship among these three equivalence relations? If every class of R_f intersects every class of R_g, and vice versa, then the observables f and g are completely unlinked. That means that knowing the value of one observable provides no information on the value of the other. In other words, the reduced state space of S/R_{fg} is the Cartesian product of the reduced state spaces generated by f and g.

$$S/R_{fg} \rightarrow S/R_f \times S/R_g$$

On the other hand, if every class of R_f intersects exactly one class of R_g, and vice versa, then the observables f and g are completely linked. Knowing the value of one observable determines the value of the other. This substantially reduces the possible state space as now

$$S/R_{fg} \subset S/R_f \times S/R_g.$$

Returning to the two-body example, imagine that the two bodies are widely separated. If the observables of interest are the positions of each body, then the two positions are unlinked. Setting the position of one body does not restrict the set of possible positions of the other. Now, assume that we also want to measure two more observables: the temperature of each body and the peak wavelength of electromagnetic radiation emitted by each body. These two observables are linked because only certain combinations of equivalence classes are allowable. For example, if the temperature of one of the bodies is 290K, the peak wavelength cannot be in the ultraviolet range. For a perfect black body, the linkage relationship is described by Planck's Law. One could argue that most, if not all, scientific laws are descriptions of linkage relationships.

This concept will be important when considering how to model a system. A linkage relationship can also be viewed as a symmetry that allows one to compress the state description of the system. Consequently, for an abstraction to be useful, it should consist of a set of observables that are related by linkage relationships. Or, to put it another way, what would be the benefit of including unlinked observables in the same abstraction? For example, it is useful to include body temperature and the intensity of emitted radiation at each wavelength in the same abstraction. One can use the linkage relationship to build an infrared thermometer for instance. But there would be little use to including an unlinked observable like position in that abstraction.

More generally, two or more observables may be partially linked where knowledge of the value of one observable provides incomplete information on the state of another. For example, the object might not be a perfect black body. Linkage relationships may also involve more than two observables. An example of this would be Ohm's law (*V=IR*) which assumes a complete linkage among the observables voltage, current, and resistance in an electrical circuit. Knowing values of two of the observables enables us to determine the third. Importantly, the strength of a linkage relationship among observables may vary over different subsets of the state space, *S*. This is true of most if not all of the scientific laws observed to date. Thus, one must always specify when a given law or symmetry relationship does and does not apply.

6.3.3 HOW DO WE MODEL A PERSPECTIVE OF A SYSTEM?

Symmetry relationships also enable us to build models of a system. As a term, model has many different uses in many different contexts. Consequently, we must define what we mean by model in the context of this discussion acknowledging that this definition is not universal. In the discussion that follows, we will limit the scope to models that we use for prediction as that is chiefly the motivation behind the model composition efforts in engineering.

In short, prediction is the ability to determine the state of a system of interest under circumstances not experienced including different times, locations, and contexts. One way this could be accomplished is with a complete description of all possible state transitions for a system of interest. In terms of the setup developed in the previous section, this would be the automorphism that generates the dynamics of the system.

$$S \xrightarrow{T} S$$

There are two problems here. First, we do not know what *S* is as we interact with it indirectly via meters. Second, even if we knew what *S* was, for any non-trivial system, determining all the state mappings is effectively impossible since one will not or cannot experience all possible states $s \in S$. So what are we left with? As discussed in the previous section, we can achieve a reduced description of the state space *S* through observables. So the next best thing is if we could identify an endomorphism (T_F) over the reduced state space for a set of observables, *F*, that we are interested in.

$$S/R_F \xrightarrow{T_F} S/R_F$$

The objective is to infer the dynamics of the reduced set of states of the system by taking successive readings with meters. Again we are faced with the problem that predicting the future state of a system of interest involves explicitly knowing all possible state transitions for the reduced state space.

One way to address this problem is to find a relationship among the observables that is invariant over the dynamics. A symmetry relationship fits this requirement. A symmetry allows one to compress the mapping by dropping redundant relationships. They can be reconstructed

from the symmetry relationship when needed. By selectively applying these symmetry relationships, one can build a new system (physical or mathematical) that can serve as a compressed representation of the target system's behavior. We call this new system a model for the target system. In other words, the symmetry relationships are used to reconstruct the target system's dynamics on demand via the execution of experiments for physical models or computation for mathematical models.

In order to make this concept precise, we need to introduce a new set of states for the system we are calling our model of $(S/R_F, T_F)$. Let X be the set of states of this new system with a corresponding set of allowable state transitions, D_X. For the system (X, D_X), to be a model of the dynamics of abstraction of the system S/R_F, Equation 2 must commute.

$$
\begin{array}{ccc}
S/R_F & \xrightarrow{\ T_F\ } & S/R_F \\
{\scriptstyle \alpha}\downarrow & & \downarrow{\scriptstyle \alpha} \\
X & \xrightarrow{\ D_X\ } & X
\end{array}
$$

Equation 2

In essence, what this diagram asserts is that if we measure the observables of interest on the system, encode them into the state space, X, of the model via the mapping α, and propagate the model state forward using the mapping, D_X; we will get the exact same result as if we measure the system at the later time and mapped it into the model via α. This definition is quite general. (X, D_X) could represent a physical analog or a mathematical model. If this diagram commutes, repeated applications of D_X given a particular starting state yields the predicted trajectory of the system through the state space.

More precisely, X, is the encoding via the mapping α of a subset of the state space $\prod_{f_i \in F} S/R_{f_i}$. This reduction is achievable because of the identified linkage relationships among the variables. In the case of a mathematical model, X captures the equation of state. We should note that any observables in the original set, F, that are completely unlinked with the observables of interest are typically omitted. Mathematically, this is equivalent to replacing these with constant observables. In the case that we also restrict the state space, S, such that it falls entirely within a single equivalence class of another observable, that observable can be viewed as a parameter of the model.

The interpretation of D_X, depends on whether X is a physical analog of the target system or a mathematical model. In the case of the former, we induce some physical analog of the dynamics. An example would be testing a model aircraft in a wind tunnel. In the case, of the latter D_X takes the form of computation, which could be solving an analytical model or running a simulation.

Returning to our two-body system, one example of a model of the positions of this system over time could be $(x_i, dx_i/dt)$ where x_1 and x_2 are the positions of the two bodies. If the two bodies are far enough apart, we can treat the gravitational force as negligible and model the state transitions of the two bodies independently using $(x_i, dx_i/dt)$ where x_1 and x_2 are the positions of the two bodies. If this is a valid model, then we should expect our predictions of positions at future times generated with our mathematical model to match the measurements taken on the real system. That is effectively what Equation 2 asserts.

The reader may note that if the dynamics of the system is stochastic, (i.e., T_F is not one-to-one), then the diagram will not commute. Of course, if the diagram does not commute, then (X, D_X) is not particularly useful as a model. This is addressed in stochastic models by treating the observables exhibiting stochastic behavior as probability distributions. In other words, the observable of interest is converted from a point value on the real number line to a function. This restores the commutativity of the diagram and makes the model deterministic over this adjusted set of observables. For example, if a weather model predicts temperature, one would want the model to generate the same distributions of temperatures as is observed in the real weather system of interest. Another example is quantum mechanics. The propagation of the wave function is completely deterministic. It is the specific point measurement that is probabilistic. This is known as collapsing the wave function.

6.3.4 WHAT ARE THE RELATIONSHIPS AMONG MODELS OF DIFFERENT PERSPECTIVES?

Most models of real world systems are composites. Why? The scientific laws we work with, whether Newton's Laws or the law of one price, are only applicable under a specific set of circumstances or assumptions. For example, Newton's law of gravity determines the strength of the gravitational force between two point masses. What happens if there are more than two point masses? The presumption is that we can reduce the system to pieces where the law or symmetry relationship applies, then put the pieces back together again to obtain the behavior of the whole system. This is essentially the definition of reductionism.

In terms of our setup, this means we break the observables up into groups and work with the groups separately. In the two-body example, the positions of the two bodies are completely unlinked if they are far enough apart that gravitational attraction is negligible. Thus, the trajectories can be generated separately while still obtaining the correct position of each body. The model is technically a composite, but the composition is fairly straightforward.

Of course, this is not generally the case, which is why most modeling is a little more complicated than this. As explained in the previous section, modeling a subset of the observables implies that the omitted observables are constant. If these omitted observables are unlinked with those retained in the model, then it is not a problem. However, if the omitted observables are not totally unlinked, the composition of the partial models yields a state space that does not completely correspond with the state space of the real system. Mathematically, the state space of the composed model will be larger than that of the real system. For example,

for two sets of observables *F* and *G*, the state space of the composed model is $S/R_F \times S/R_G$, of which S/R_{FG} is only a subset (Rosen 1978). We have no way to know which states of this enlarged space are real and which are artifacts of the composite model.

For the two-body example, there are two additional cases of interest. 1. the bodies are close enough that gravitational attraction matters, and 2. the bodies are colliding. Both involve linkage relationships, but, as a practical matter, each is handled differently. In the first case, we can compute the instantaneous acceleration due to gravity and propagate the system over small time steps. In the second, we must find a simultaneous solution for multiple symmetry relationships including conservation of momentum and conservation of energy. Rosen makes no distinction among such cases, as his interest was exploring relationships between physics and biology. However, for engineering modeling, the distinction matters. Consequently, the next section will explore the differences in more depth.

6.4   ANALYSIS OF MODEL COMPOSITION

With the basic mathematical machinery in place, we now consider the implications of composing multiple models, each based on a different abstraction. More specifically, if a composition is successful, what does it imply about the system itself and the models that describe it? We will start by extending the definition of a valid model from the previous section to accommodate a composite model and identify the implied conditions. We then consider the impacts of violating those conditions on achieving a successful composite model.

Since we are considering composing multiple models based on different abstractions, we need to define each model. First, partition the set of observables *F* into *n* subsets G_i. Applying any one set of observables to the system yields the abstraction S/R_{G_i}. To capture the dynamics under this subset of observables, we need to project the dynamics T_F into the subspace S/R_{G_i}. We will call this projection T_{G_i}. This results in the reduced description of the system $(S/R_{G_i}, T_{G_i})$. Consistent with the previous section, a model of the reduced description is (X_i, D_i).

Imposing the condition that the diagram in Equation 2 must commute for (X, D_X) to be a model of the system $(S/R_F, T_F)$, then model composition can be viewed as the situation where $(S/R_F, T_F)$ has been projected into multiple subspaces $(S/R_{G_i}, T_{G_i})$ which are each modeled individually as (X_i, D_i) then composing those models to yield (X, D_X) while preserving the commutativity of the diagram. For two models, Equation 3 must commute.
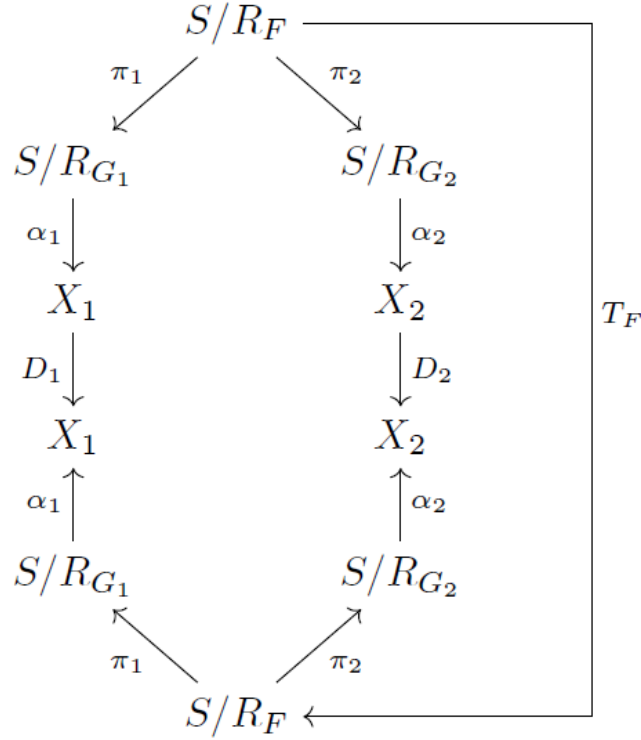
Equation 3

Note that this diagram is a modification of Equation 2. The difference is that there are two models operating in parallel. One can take the set of observables, F, project it into two different views of the system using the subsets of observables G_1 and G_1 via the natural projections π_1 and π_2, model and propagate each view separately and still yield the same result as measuring the state of the system again at the later time. For the remainder of this paper, we will limit the commutative diagram to two abstractions, but it should be obvious how they could be extended to include models of more than two abstractions.

The first observation that we will make is that for this diagram to commute, the abstractions S/R_{G_1} and S/R_{G_2} must be unlinked. If there are any linkage relationships among the observables then there are restrictions on the allowable states or state transitions that are not captured in one or both models. Consequently, the combination of the models (X_1, D_1) and (X_2, D_2) could achieve a combination of states not allowable in S/R_F.

To make this more concrete, consider the simple two-body example. For the case where the two bodies are widely separated and gravity is negligible, the dynamics of each body can be modeled independently, because the position of one has no impact on the position of the other. They are unlinked and the models would satisfy the Equation 3. However, if the bodies are close enough that gravity is a factor, then these independent models are no longer valid. Gravity creates a linkage relationship among the otherwise independent projections. Running

the models independently would result in a combination of states that is not achievable in the real world. Equation 3 would not commute.

Is there a way to accommodate this linkage relationship? Consider how one might model the two-body problem with gravity. As $\Delta t \to 0$, the state transition is governed by the instantaneous acceleration due to gravity,

$$\frac{d^2 x_i}{dt^2} = \frac{Gm_j}{(x_i - x_j)^2}.$$

Thus, the state transition for body i is determined by a combination of state information from both bodies $(x_i, x_j, x_j, v_i) \to (x_i, v_i)$. The mass and position of the other body are effectively parameters in the model. As a result the trajectories of the two bodies can be modeled using two different models as long as state information is exchanged between the two at short time intervals.

Equation 3 will not commute because D_1 and D_2 will not be functions. Since any given $x \in X_i$ does not uniquely determine the subsequent state, $D_i(x)$ may map to more than one future state. In essence, the state information from the other model serves as parameters for D_i. So while one cannot run truly independent models, the state transitions can still be computed independently as long as state information is coordinated. More formally, Equation 4 must commute.
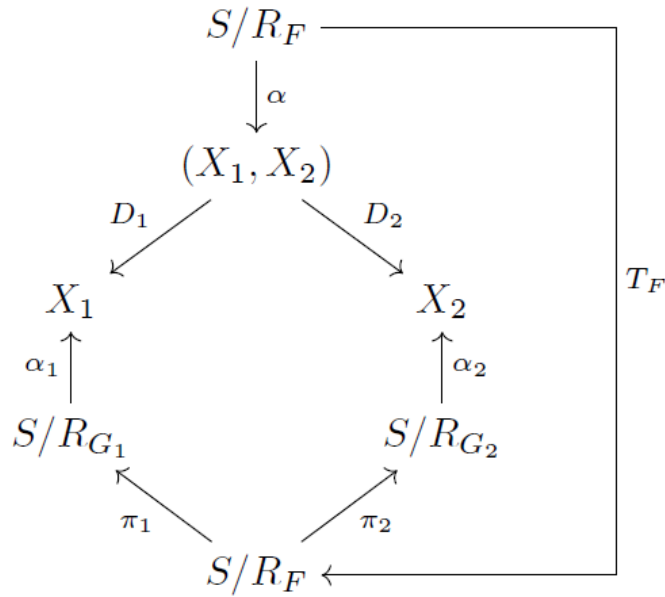
Equation 4

Note that the major difference between Equation 4 and Equation 3 is that the parallel paths for encoding the model state information have been collapsed into a single path. Since the states

of one abstraction serve as parameters for the state transition for the other, it is no longer valid to project the system into separate subspaces then map to the model states as the necessary parameter values would be lost. However, that information is not required when checking the correspondence of the models with the true system after state transition. That is why the bottom of the diagram remains the same, and we are able to maintain separate D_i's. That allows one to have separate dynamic models for each subset of observables. In this case, we will call the models state linked because they must exchange state information.

However, we should note that Equation 4 implies that all combinations of states from S/R_{G_1} and S/R_{G_2} are still allowable. For example, setting the position for one body does not intrinsically restrict the set of possible positions where we can place the second body. If there are linkage relationships among the observables of the two abstractions that limit the allowable combinations of states, then Equation 4 will not commute.

Assume that the two bodies are colliding. This means that conservation of momentum and energy apply. For instance, $m_1 v_1 + m_2 v_2 = C$ must hold both before and after the collision. This means that post-collision velocities cannot be determined independently. For a perfectly elastic collision, one would need to find a solution that simultaneously satisfies the equations both for the conservation of linear momentum and the conservation of kinetic energy. Certain combinations of velocities are not allowable.

In such a case, the parallel paths of Equation 4 must also be collapsed into a single path because certain combinations of observables are not allowable. Thus, projecting the system into two independent subspaces would allow infeasible combinations of states. This, in turn, collapses the two transition mappings D_1 and D_2 into a single mapping because some combinations of elements of D_1 and D_2 are forbidden. At this point, independence between the models is lost, and there is really only one model. This is evident in Equation 5. In this case, we will call the models transition linked because they must coordinate state transitions.

$$
\begin{array}{c}
S/R_F \\[4pt]
\alpha \downarrow \\[4pt]
(X_1, X_2) \qquad T_F \\[4pt]
D \downarrow \\[4pt]
(X_1, X_2) \\[4pt]
\alpha \uparrow \\[4pt]
S/R_F
\end{array}
$$
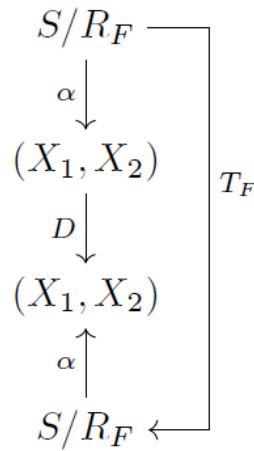
Equation 5

This analysis leads us to define three types of linkage relationship for the purpose of engineering model composition:

- *Unlinked* - there is no relationship among the subsets of observables of the various subsystems

- *State linked* - Any combination of states among the subsystems is allowable, but that combination affects the state transition behavior of each subsystem. Consequently, each model must know something about the states of the others.

- *Transition linked* - Not all combinations of states among the subsystems are allowable. Consequently, the transition behavior of all states must be determined simultaneously.

It should be noted that these diagrams are not intended to be representative of how one would actually build the model. Rather they express the mathematical conditions that must be met if one wanted to build a composite model. While developing composite models that meet these requirements may seem obvious for the simple two-body example, it is not so obvious when considering multiple engineering models capturing different abstractions of the same entity, for example, aerodynamic and thermodynamic models of the same aircraft.

From an engineering standpoint, the interesting case is treating a set of transition linked models as state linked. This can occur when one attempts to compose two models by coordinating data exchange and synchronizing execution without realizing that there is a latent transition linkage. As shown above this would allow the models to achieve impossible states. Returning to the two body example, this would be equivalent to not checking the conservation of momentum condition after the collision.

6.5   INSIGHTS FROM MULTISCALE PHYSICS MODELING

It has long been recognized in physics that systems will exhibit qualitative differences in behavior at different spatial and temporal scales (See Section 5.1). As a result, different sets of observables (i.e., abstractions) are applicable at different scales. Thus, one may model a solid object as either a continuum or a discrete set of particles depending on the circumstances and question of interest. As long as a given question can be answered with a single abstraction, we do not have to worry about model composition. However, there are many questions that arise in engineering and physics that cannot be addressed with a single abstraction either because of issues of computational tractability or because no one abstraction can capture the phenomena of interest. Addressing such situations is the domain of multiscale physics modeling.

Hoekstra, et al. (2014) provide a recent overview of the state of the field. A central aspect of multiscale modeling is what they call scale bridging. Winsberg (2010) considers this problem in depth. He highlights two approaches: serial multiscale and parallel multiscale. Serial multiscale

is the most common and describes the case where we run a model at one scale first, and then use it to parametrize a model at another scale. Parallel multiscale modeling is the case where the abstractions at different scales interact and consequently, the models cannot be run sequentially. They must be run in parallel. We will argue that these two approaches correspond with the state linked case and the transition linked case respectively.

Yang and Marquardt (2009) present a set theory based characterization of multiscale modeling and attempt to capture both cases. However, their formulation implicitly relies on the reductionist hypothesis. That is the system can be decomposed into a hierarchy of subcomponents. While this may be an acceptable assumption under some circumstances, it is questionable in the general case. As argued by Pennock and Gaffney (2016), regardless of the veracity of the reductionist hypothesis, as a practical matter we must contend with multiple overlapping and incompatible ontologies when we consider a system from multiple views.

To this point, Winsberg considers the real world case of researchers attempting to build a physics-based multiscale model of nano-crack propagation in silicon[14]. In short, to model the phenomenon, one must simultaneously consider linear-elastic theory, molecular dynamics, and quantum mechanics. The problem is that these three theories are inconsistent and incompatible. To make the simulation work, "handshaking algorithms" that require deliberate fictions must be introduced to translate parameter values back and forth among the three views. For instance, fictitious "silogen" atoms are introduced on the boundary between the molecular dynamics view and the quantum mechanical view. There is no such thing as a silogen atom, but it serves the purpose of passing state information between the incompatible views in a manner that makes the state transitions for both views feasible. However, Winsberg also notes that these linkage relations have an empirical aspect. This would seem to be consistent with observations that scale bridging approaches tend to be domain and/or application specific (Hoekstra et al 2014, Chopard et al 2014).

These observations are also consistent with our discussion of Equation 5 where there are transition linkages among the abstractions. In the example above, researchers are modeling the exact same block of material as a continuum, molecules, and quantum particles simultaneously. However, when one creates three independent models, latent linkages among these views are lost. Consequently, the composite model can achieve states that are not achievable in the real system. The state restrictions must be built back in somehow. That is the role that these "fictions" play. However, since they are not always derived from theory, they must be developed via trial and error and will likely be application specific.

Let us now consider how these workarounds from multiscale physics fit into our mathematical formulation of multi-modeling.

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[14] The original work is documented in Abraham et al (1998).

6.5.1 WORKAROUNDS FOR STATE LINKAGES

First, consider the case of serial multiscale modeling. This is effectively a variation of the two-way state linkage case described by Equation 4. If one can assume that this linkage is one-way, that is the state propagation of one abstraction depends on the state of the other, but not the other way around, then the diagram shown in Equation 6 commutes.

$$
\begin{array}{c}
S/R_F \\
\pi_1 \swarrow \qquad \searrow \alpha \\
S/R_{G_1} \qquad\qquad (X_1, X_2) \qquad T_F \\
\alpha_1 \downarrow \qquad\qquad \downarrow D_2 \\
X_1 \qquad\qquad X_2 \\
D_1 \downarrow \qquad\qquad \uparrow \alpha_2 \\
X_1 \qquad\qquad \\
\alpha_1 \uparrow \qquad\qquad \\
S/R_{G_1} \qquad\qquad S/R_{G_2} \\
\pi_1 \searrow \qquad \swarrow \pi_2 \\
S/R_F
\end{array}
$$
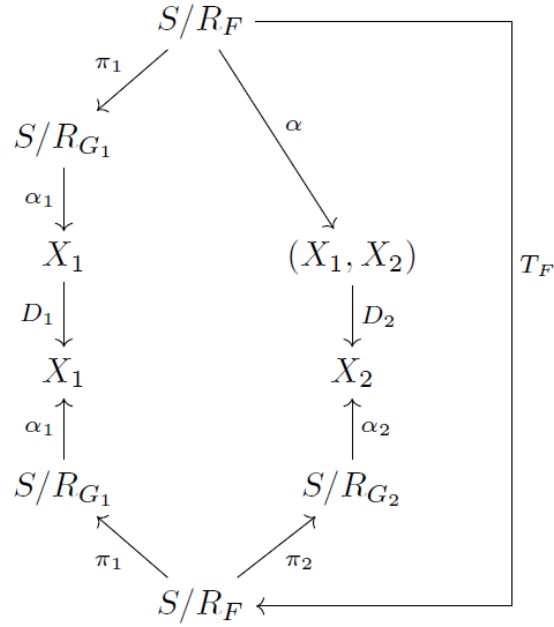
Equation 6

At first glance, it might seem that there is no gain from decomposition since the state space for S/R_{G_1} is encoded in the model for S/R_{G_2}. However, meeting this requirement allows one to decouple the dynamic propagation of S/R_{G_1} from S/R_{G_2} entirely. Thus, it is feasible to compute the state space trajectories for S/R_{G_1} first, then compute the state space trajectories for S/R_{G_2}, using the precomputed trajectories of S/R_{G_1} as an input. A simple, non-physics example of this case is modeling the accumulation of interest in an individual's bank account. The growth in the balance is dependent on the interest rate, but the interest rate does not depend on the current bank balance. Thus, one can create a model to forecast future interest rates and then feed the results into the bank account model.

6.5.2 WORKAROUNDS FOR TRANSITION LINKAGES

While it was shown in previous sections that, in the most general case, abstractions that are transition linked require an integrated model, the work in physics-based parallel multiscale modeling suggests that there might be special cases where one can work around this limitation. The first case is when there is a refinement relationship between S/R_{G_1} and S/R_{G_2}.

If S/R_{G_1} refines S/R_{G_2}, then each equivalence class of S/R_{G_1} intersects exactly one equivalence class of S/R_{G_2}, but any given equivalence class of S/R_{G_2} may intersect more than one class of S/R_{G_1}. This is an aggregation relationship between S/R_{G_1} and S/R_{G_2}, which is equivalent to a one-way transition linkage. Consequently, the two abstractions are compatible, and the linkage relationship is known, but S/R_{G_1} allows one to resolve more system states than S/R_{G_2}. Thus, one could view it as a higher resolution model. Under these circumstances, one can run the model (X_1, D_1) first. Then use it to parametrize (X_2, D_2), which is run second. This illustrates case of multi-fidelity modeling where one conducts a limited number of runs of the high fidelity model to calibrate a lower fidelity model that is used to explore a larger space. This situation is analogous to that presented by Yang and Marquardt (2009).

The second case is where there is no refinement relationship between the abstractions as was the case with the nano-crack propagation model. To convert the transition linkage to a state linkage, one can partition S into multiple subsystems. For two parallel abstractions, create three subsystems, S_1, S_2, and S_3, by employing the subset of observables G_3. A spatial division is a good example but not strictly required. The idea is to apply abstraction G_1 to S_1 and abstraction G_2 to S_2. Because the abstractions G_1 and G_2 are applied to non-overlapping subsystems, there is no longer an implicit transition linkage.

This is depicted notionally in Figure 10. Here, G_3 is a single, real-valued function. A threshold k converts the S into three subsystems S_1 $(G_3 < k)$, S_2 $(G_3 > k)$, and $S_3(G_3 = k)$. However, this creates two issues. First, since no abstraction is applied to S_3, the state information about this portion of the system is lost. Second, the state transition behavior of S_1 is affected by the state of S_2 and vice versa, but the state transition for S/R_{G_1} is incompatible with S/R_{G_2} and vice versa. The first issue is addressed by making S_3 as small as possible. The second issue is addressed by introducing Winsberg's fictions. In essence, S_3 is represented by an artificial abstraction.
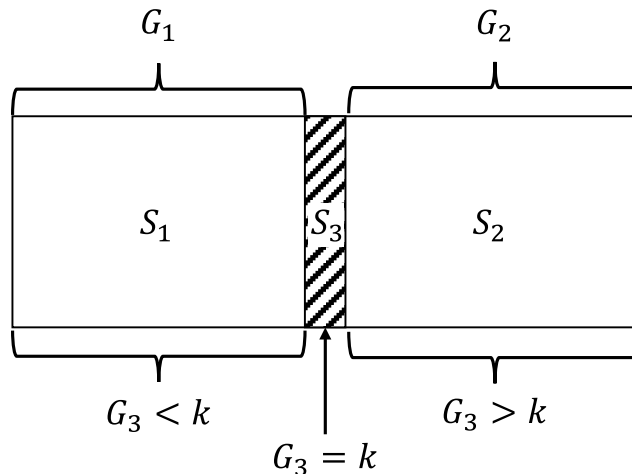
Figure 10 - Notional partition of the system S/R_F into non-overlapping abstractions $S_1/R_{G_1G_3}$ and $S_2/R_{G_2G_3}$ using the observable G_3

In Winsberg's example, the fictitious "Silogen" atoms on the boundary between the region modeled using molecular dynamics and the region modeled using quantum mechanics serve as the artificial abstraction. The net result of this approach is a more accurate model of the whole system at the price of lost information about overlap region. As long as the overlap region is small, this can be an acceptable price to pay.

Since this "workaround" converts transition linked sets of observables into state linked sets, the resulting requirement is a modification of Equation 4. First, the original state space S/R_F is converted to the partitioned state space $S_1/R_{G_1 G_3} \times S_2/R_{G_2 G_3}$ via the mapping P. Second, the "fictions" X_3 and X_4 are introduced to replace the missing state information for S_3 in a way that is compatible with each abstraction. The result is Equation 7. If this diagram commutes, one can apply a parallel multiscale model (or something analogous) to capture the behavior of the system.

$$
\begin{array}{c}
S/R_F \\
\downarrow {\scriptstyle P} \\
S_1/R_{G_1 G_3} \times S_2/R_{G_2 G_3} \\
{\scriptstyle \alpha_{13}} \swarrow \qquad \searrow {\scriptstyle \alpha_{24}} \\
(X_1, X_3) \qquad\qquad (X_2, X_4) \qquad {\scriptstyle T_F} \\
{\scriptstyle D_1}\downarrow \qquad\qquad\qquad \downarrow {\scriptstyle D_2} \\
X_1 \qquad\qquad\qquad X_2 \\
{\scriptstyle \alpha_1}\uparrow \qquad\qquad\qquad \uparrow {\scriptstyle \alpha_2} \\
S_1/R_{G_1 G_3} \qquad\qquad S_2/R_{G_2 G_3} \\
{\scriptstyle \pi_{13}} \searrow \qquad\qquad \nearrow {\scriptstyle \pi_{23}} \\
S/R_F
\end{array}
$$
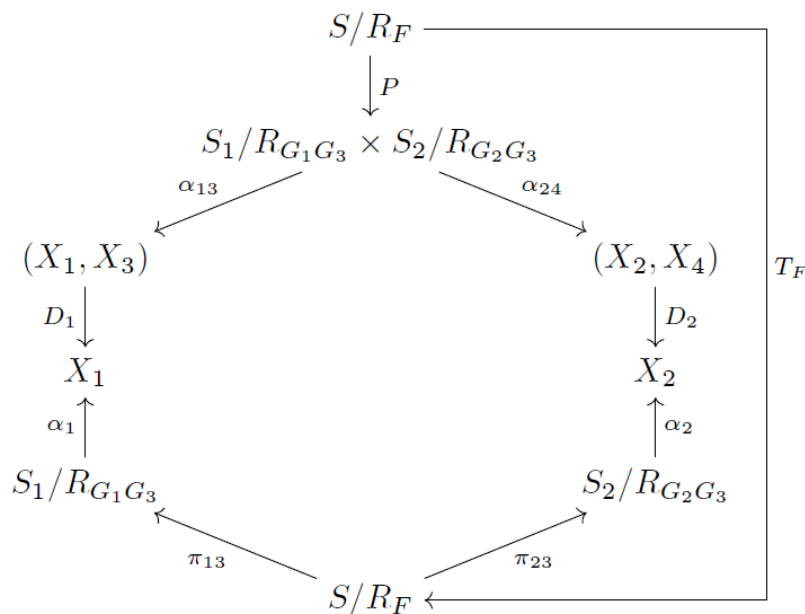
Equation 7

A few things to note: The fictions X_3 and X_4 are encoded via functions of the system state for each abstraction. Since the fictions are not always defined by a meter, their state values may not be the result of direct measurement. Instead encoding functions must be determined through trial and error. This is consistent with Winsberg's observations. The structure of the fiction would be determined experimentally, and the state of the fiction at any one instant would be determined by a combination of the states from each of the abstractions.

6.6   IMPLICATIONS FOR BUILDING ENTERPRISE MODELS

Let us revisit the questions posed earlier in light of the analysis performed. First, we can define a perspective or abstraction of a system as a quotient set determined by the selected collection of observables. Applying the quotient set definition leads to a precise characterization of the linkages among the multiple perspectives of the same system. Models of these system perspectives inherit these linkages whether recognized or not.

This leads to the obvious conclusion that a successful composition of models from different perspectives means that these linkage relationships are either absent or explicitly accommodated as failure to account for them allows the composed model to achieve unallowable states. That, in of itself, is not particularly interesting. Rather it is the subsequent characterization of models as either state linked or transition linked that is useful. It allows for a precise definition of what it means to be conceptually interoperable. If two models are conceptually interoperable, there are no latent transition linkages among their corresponding abstractions.

The justification for this definition is as follows. Obviously if two models are unlinked, there is no interoperability issue. If two models are state linked, then their composition is valid if data exchange and state transitions are synchronized. This means that satisfying levels 1 through 5 of the LCIM (technical, syntactic, semantic, pragmatic, and dynamic interoperability) is sufficient to achieve interoperability (Wang et al 2009). No additional condition is required. Thus, satisfaction of Level 6, conceptual interoperability, is implied. However, if two models are transition linked, satisfaction of levels 1 through 5 is not sufficient. Their theories are "inconsistent" which means that they lack conceptual interoperability.

Explaining a lack of conceptual interoperability as the presence of transition linkages among models, clarifies an assertion made by Wang et al. (2009) that the challenges that simulation developers have experienced when applying HLA can attributed this to a lack of conceptual interoperability among the federated simulations. If the simulation models are state linked, then a framework such as HLA should be sufficient as it coordinates execution and data exchange. However, if there are transition linkages among the models then data exchange and coordinated execution are insufficient to achieve a valid composition.

There are several observations that follow directly from the proposed definition of conceptual interoperability:

- Transition linkages may vary over different subsets of the system's set of states. Thus, two models may be conceptually interoperable under some circumstances but not others. Conceptual interoperability is not an absolute attribute of a pair of models.

- Conceptual interoperability is equivalent to the case where each transition linkage is contained within a single model.

- Transition linkages among models may be removed by either repartitioning the set of observables, *F*, into new subsets or partitioning *S* into non-overlapping subsystems using a subset of *F* as the basis for partition.

6.6.1 Sources of Transitions Linkages

In order to understand how to mitigate transition linkages among models, it is necessary to consider the sources. Four sources are hypothesized:
1. *Explicit:* The transition linkages are known in principle, but the composite model is large and complicated. Consequently, they are difficult to find and accommodate.

2. *Domain Exceedance*: The models in question are unlinked or state linked for the subsets of *S* for which they were designed, but they are unknowingly applied to a subset of *S* for which there is a transition linkage.

3. *Intentional Duplication:* *S* is intentionally modeled using two different transition linked abstractions because none of the available abstractions would allow Equation 2 to commute for the phenomena of interest.

4. *Unintentional Duplication:* A subsystem of *S* is unintentionally modeled using two different transition linked abstractions as a consequence of independent model development.

Case 1 is the domain of constraint theory (Friedman & Leondes 1969a,b,c). The necessary linkage relations are present in the models, but they have been combined in such a way that they inappropriately constrain the variable space. Constraint theory provides a means to analyze these situations.

Case 2 is a fairly common modeling problem. For example, in the two body model, a latent transition linkage would occur if one used the state linked gravity models but never checked for a collision between the two bodies.

Case 3 is exhibited in the parallel multiscale physics example. Because, none of the available abstractions could accurately model the crack propagation, the researchers combined them. Figuratively, they are modeling the same thing different ways at the same time, but they have no other choice.

Case 4 is more subtle. When modeling any system, one must often make assumptions about that system's context. If an observable of the context is ignored, then the modeler is assuming that the observable is unlinked or constant. If the linkage is recognized, then the modeler is explicitly or implicitly integrating the context into the system model.

For example, imagine two models that represent the dynamic behavior of two different projectiles. One model assumes that the Earth is flat. The other model assumes that the Earth is a sphere. However, neither model explicitly models the Earth. Rather the Earth is modeled implicitly as a consequence of the selected equations of motion. Thus, the problem may not be immediately obvious upon inspection of the models. Yet, if these two models are taken "off the shelf" and integrated into a larger model, they have implicitly modeled the Earth twice. There is a latent transition linkage that must be dealt with.

6.6.2 POSSIBLE MITIGATIONS FOR EXISTING TRANSITION LINKAGES

As noted above, removing transition linkages among models involves either repartitioning the set of observables, F, into new subsets or defining subsystems of S using a subset of F as the basis for partition. Depending on the circumstances, only one of the approaches may be viable. When both choices are available, there are tradeoffs. Repartitioning F is tantamount to redesigning the models to ensure that the transition linkages are contained within integrated models. Partitioning S, on the other hand, requires the introduction of "handshake algorithms" or "middleware." As noted by Winsberg, developing these may require trial and error, particularly when there is no theoretical explanation of the relationship. When trial and error is necessary, the resulting ``handshakes'' are effectively empirical. It is tantamount to interpolation over the available data set. Thus, one must be concerned with the risk of model induced error when predicting the consequences of a design decision outside of the training data versus when a fully unified theory is employed. Real world modeling efforts may face transition linkages from multiples sources, thus, it will likely be a case-by-case decision.

The author considers the first two cases to be instances of common problems faced when composing engineering models. Thus, the proposed solutions are "standard" to some extent. This is not to suggest that they are easy problems to address. Rather, there is already much work going on to address these. Consequently, the proposed mitigations are only discussed briefly for completeness. The author's hypothesis is that the second two cases are major challenges to MBSE and MCE approaches. The hypothesized approaches for addressing transition linkages among models for each source are summarized in Table 4.

Table 4 - Hypothesized Approaches for Addressing Transition Linkages

Linkage Source	Preferred Approach	Supporting Methods
Explicit	Partition F	Use domain ontologies combined with formal model checking procedures
Domain Exceedance	Partition F	Use documentation of domain constraints with formal model checking procedures
Intentional Duplication	Partition S	Partition S into non-overlapping subsystems and use empirically calibrated "middleware" to bridge the partitions

Unintentional Duplication	Partition *S*	Use domain ontologies and testing to identify potential linkages. Then partition the *S* into non-overlapping subsystems

As mentioned previously, Case 1 is addressable via constraint theory. Since the linkage relationships are explicitly known, repartitioning *F* and developing integrated models may be the preferred approach. Model documentation, formal domain ontologies, and formal model checking procedures may assist modelers with this assessment.

Similarly, the preferred solution for Case 2 is to repartition *F* when the necessary linkage relationships can be introduced. To facilitate such assessments, metadata describing the conditions under which the model is valid could be useful. However, there are limits as it is effectively impossible for model developers to list every factor that they did not consider. This problem is exacerbated when certain model formulations are standard for a domain and the model developer may not even be aware of its limitations. Again, domain ontologies and formal model checking procedures may be helpful in identifying these linkages.

For case 3, the only real option is to partition *S* as was done in the crack propagation example. This involves choosing a set of observables to break *S* into non-overlapping subsystems. The common basis for partition will likely be spatial for most engineering problems. Once the partition is created "middleware" or "handshake" algorithms can be developed to transfer state information across the partition. This effectively converts the transition linkages into state linkages.

For case 4, there are no obvious answers. This case would typically arise in situations where one wants to reuse existing models and simulations, but they are black boxes. If that is the case, partitioning *S* may be the only viable option. Domain ontologies may aid in identifying typically assumed objects and relations for a given application area. This may support targeted testing and evaluation of a candidate model to infer how relevant phenomena were implicitly modeled. For example, if a domain ontology or other documentation indicated that there is relationship between the projectile and the Earth, this could cue a modeler to evaluate a candidate model to infer the assumed representation of the earth: flat, spherical, oblate spheroid, etc. If a duplicate representation is detected, it may be possible to handle it via partitioning of *S*, but it may require trial and error to develop a calibrated "handshake" among the partitions.

6.7   IMPLICATIONS FOR MULTI-LEVEL MODELING

Reflecting on the four sources of transition linkages and the associated mitigations, there are several implications for building a composite model from multiple existing models or theories. If the sources of transition linkages among candidate models are limited to cases 1 and 2, then methods commonly suggested to facilitate model interoperability including ontologies, model

metadata, and formal model checking procedures may be effective. (This is analogous to MDO.) However, two aspects of multi-level modeling that risk triggering case 3 and case 4 sources of transition linkages. The first is the necessity of employing multiscale ontologies. This runs immediately into case 3, which means that "handshake" algorithms will be required and these may be empirical and case specific. The second is the desire use off-the-shelf models in a "plug and play" fashion. Because off-the-shelf models may have been designed for any number of purposes, then case 4 sources of transition linkages are likely. Again, addressing these may require case specific "handshake" algorithms.

The case 3 issues are fundamental, and only new scientific theories can permanently resolve them. This leaves modelers with problem or domain specific solutions. The case 4 issues may also be resolvable in a problem or domain specific way, but this defeats the intent of general "plug and play" model composition. Note that all of the approaches to mitigating transition linkages among models are more tractable in a stable problem space. This would be consistent with assertions that multi-scale modeling is more likely to be successful when domain focused.

This is to be expected because an unmodeled transition linkage is essentially information about the system that is lost as a part the reduction process. To account for the linkage, that information has to be put back in the model. Thus, experience acquired through trial and error serves as a basis for restoring the missing information. However, this is essentially an exercise in interpolation. Thus, applying the composed model outside of the experience base incurs substantial risk of model induced error.

Still, even in domain focused situations, there are likely approaches to model development and model selection that would reduce the risk of unmanaged case 4 linkages going forward. The analysis presented here leads to several research questions toward that end:

- Are there indicators that could be used to identify which analysis efforts would be at risk of incurring case 3 and 4 linkages before attempting to build a composed model?

- Are existing methods of designing for model reusability effective at minimizing case 4 linkages?

- What is the appropriate level of abstraction to target interoperability standards and tool development to minimize the risk of case 4 linkages?

    o Is the appropriate level of abstraction domain specific?

    o Would Doyle and Csete's (2011) advocated "bowtie" architectural approach to reuse help reduce case 4 linkages?

- Are there certain levels of abstraction that are less prone to case 4 linkages? Does this explain why certain software tools seem to be extremely reusable while others are not?

6.8 EXTENSIONS TO CATEGORY THEORY

One of the challenges of the problem formulation in the previous section is that it is difficult to apply the principles to more than two models in a practical sense. For example, if one wanted to compose four models instead of two, one would need to check for transition linkages for each pair of models, resulting in six comparisons. As the number of models increases, the number of required comparisons increases rapidly. For instance 5 models would require 10 comparisons and 10 models would require 45 comparisons. This does not even account for making the models mutually compatible if transition linkages are found. This is a serious impediment to implementing a practical model composition and switching approach to support enterprise modeling.

One promising avenue to address the problem is the application of a branch of mathematics called category theory. While category theory will not tell you how to eliminate the transition linkages among models, its capability to support abstraction could provide the ground rules for proper model composition and a way to reduce the number of comparisons required as each new model is added to the enterprise analysis inventory.

One way this might work is demonstrated by Wisnesky et al (2017). They apply a category theory based query language they call FQL to show how heterogeneous databases could be integrated without performing an exhaustive number of comparisons. In a sense, once two databases are combined they become a new database. So when another heterogeneous database is introduced, it only needs to be compared to the new database not the original two. This problem is analogous to the model composition problem. Of course there are some caveats and technical issues here, but it is still a promising direction of future research.

One additional feature of category theory is that it may serve as a convenient language to describe and manage heterogeneous models. This has been recognized by both Rosen (1978) and Baez and Stay (2010). The reason is that in naturally incorporates the idea of abstraction and focuses on the relations among abstractions rather than the internals of the abstraction. Consequently, one can naturally build networks of categories that are created by adding and removing assumptions (axioms) from categories. Adding and removing structure from models is analogous. Again category theory will not do the work for the modeler, but it may provide a powerful language to describe problems, establish necessary conditions, and organize models. To put it another way, category theory, by itself, provides no information about the real world. However, it may provide guidance as to how to organize information about the real world in an intelligent way. While much research is still needed to determine whether not category theory will be useful in a practical sense, it did provide the inspiration for the approaches proposed in Section 7.

7 APPROACH FOR IDENTIFYING AND COUNTER-INTUITIVE POLICY IMPACTS

Let us recap the analysis to this point. The identification of unintended policy consequences in an enterprise system will like require the systematic exploration of alternative model structures

that likely use overlapping and possibly inconsistent abstractions (ontologies) that may exist at different scales. The previous section identified transition linkages among these abstractions as an inhibitor to composing the associated models. One source of these transition linkages is overlapping representations, which is almost by definition the motivation behind multi-level modeling. Thus, a literal implementation of multi-level models where we swap different models in and out for each layer is infeasible. This was observation was also made during RT-138 (Pennock et al 2016), but now there is a mathematical explanation for this phenomena.

Reflecting on the literature review, we now see the mathematical analysis presented in Section 6 also provides a mechanism to describe, at least a high level, the differences in approach between the physical sciences and the social sciences. Essentially, when faced with a situation where no one available abstraction can explain a phenomenon, the physical sciences partition *S* and the social sciences refactor *F*. This also provides some insight into why ontologies tend to proliferate in the social sciences. This means that any systematic approach to varying enterprise model structure must explicitly account for both possible approaches to removing transition linkages.

In this section, we first describe the implications of the two approaches to removing transition linkages and the resulting implications for how enterprise models should be built, analyzed, and used. Once that is established, we consider the implications for model validation. Finally, we present a tentative approach to systematically navigating the space of possible models.

7.1   A SYSTEMATIC APPROACH TO ENTERPRISE MODEL DEVELOPMENT

7.1.1   LIMITATIONS OF EXISTING APPROACHES

Before developing a systematic approach to enterprise model development, it is necessary to consider how models are built across multiple overlapping abstractions today. Based on the analysis of the literature (Section 5), we contend that there are really two basic approaches, though actual model implementations may mix the two. First, we will consider the typical multi-scale modeling approach form the physical sciences. A notional illustration of this process is described in Figure 11.

a)

b)

c)

$$f(x, y, z) = w$$

$$g(a, b) = c$$

$$h(d, e) = f$$

d)

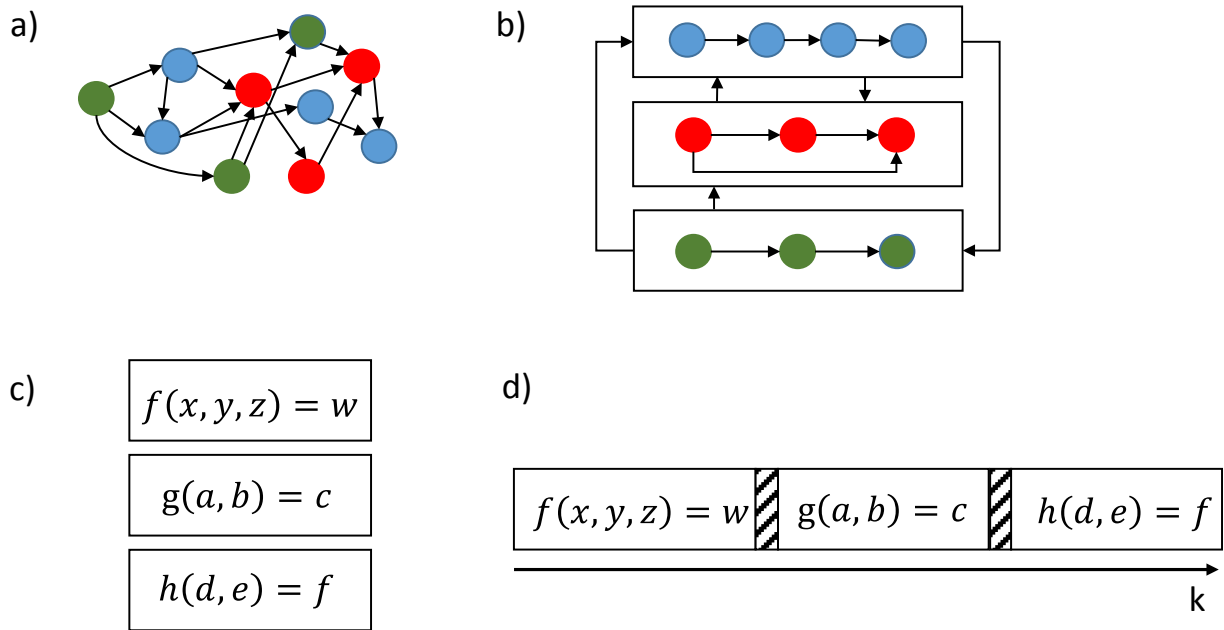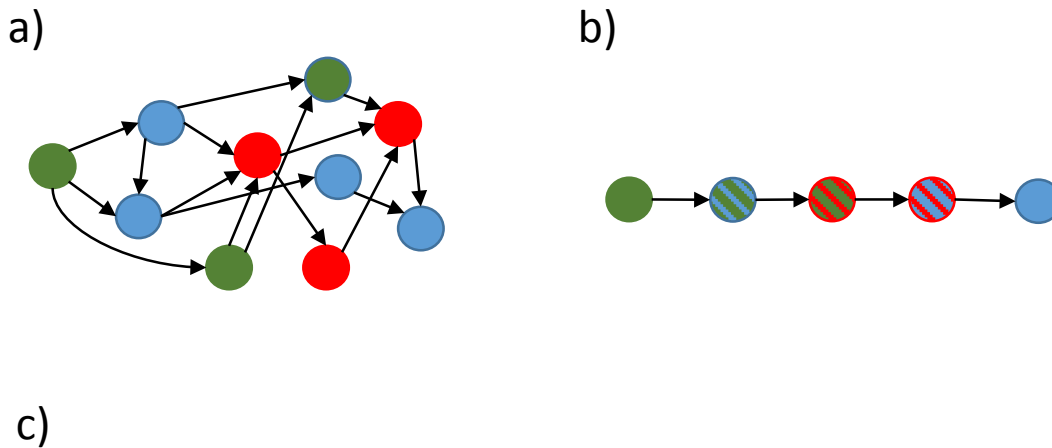$$f(x, y, z) = w \quad g(a, b) = c \quad h(d, e) = f$$

k

Figure 11 – Approach 1: a) Initial conceptualization of the system will likely involve mixtures of many factors and relationships from different absractions. b) Certain abstractions, often those defined by scientific theories, are very well understood and predictable in isolation. A natural organizational scheme is to sort the factors from the intial conceptual model into abstractions defined by theories. When these abstractions overlap, it is natural to organize them into levels. This often done by spatial scale, but that is not strictly required. c) Since the conceptual model is now organized by abstraction, there is often a natual mapping of each level to a canonical mathematical or computational model. However, this creates an issue. There may be no obvious or even theoretically backed way to relate the canonical models of the three layers. There is lost information. d) In multi-scale modeling, the system is partitioned into zones and each model applies to a different zone. However, this creates mismatches on the boundaries that must be rectified using empirical data.

First, a conceptual model of the system is built. There are many possible ways this may be done including influence diagrams, causal loop diagrams, and systemigrams just to name a few. The important thing is that potentially relevant objects and the relationships among them are identified. At this stage, the objects may be vague, come from traditionally different or even incompatible ontologies. In order to build a useful model, one must make use of symmetries. In the physical sciences in particular, these symmetries have been grouped into theories that provide useful, tested ways to represent certain phenomena. Thus, the goal of the modeler is to reorganize the mixture of objects into well-defined groupings, where each grouping is associated with a conventional abstraction and theory. If this can be done, there are often well defined and developed modeling approaches to represent each grouping in isolation. The problem is that now we may have multiple groupings. If there are no transition linkages among the groupings then one may be able to proceed with model integration at this point. However, as we saw in the multi-scale literature there are some problems where there are overlapping representations. These create transition linkages among the models that must be removed. The typical approach in multiscale modeling is to partition the system such that a different model applies to each region. However buffers are often introduced and empirical "handshake algorithms" must be developed. Thus, while each of the individual models may be well validated, this validation does not automatically pass to the composite model.

Next, we consider a refactoring approach more typical to the social sciences and some engineering applications. A notional illustration is provided in Figure 12. As with the previous case, we start with a conceptual model of the system. In this case, however, the objects may not map cleanly into well-established abstractions. Consequently, the modeler refactors the objects and relationships until a single abstraction is created. This is likely done through combination of several mechanisms. The most obvious is dropping objects and relationships that may be deemed either unimportant or that are too difficult to handle. It may also involve replacing or merging objects and relationships with approximations that are more compatible with other objects in the model. Finally, in the most extreme case, the modeler may create new objects and relationships from empirical data (see LVT analysis in Section 5.2). Once this "refactoring" is complete, the transition linkages have been managed, and the modeler has created a single internally consistent abstraction. The problem is that this "new" abstraction is essentially untested. Any standard abstractions or theories that may have applied to the original conceptual model may have been altered. Thus, as with the previous case, we have created a validation issue, and it is unclear to what extent the predictions of the model can be trusted.

a)

b)

c)

$$s(d, l, m, n) = w$$

Figure 12 – Approach 2: a) Initial conceptualization of the system will likely involve mixtures of many factors and relationships from different absractions. b) Since the abstractions are not necessarily compatible, the modeler modifies the factors and relationships to create a conceptually consistent model. This may be accomplished through a combination of dropping factors, creating approximations, selecting alternative representations, etc. c) Since there is now an internally consistent conceptual model, it can be represented using a single, consistent mathematical or computational model. However, the process of modifying the conceptual model likely lost information contained in the orginal abstractions. Consequently, the "refactored" model should be compared to empircal data and adjusted to compenstate for lost information.

In both cases we correct the compatibility problems by fitting to data, but in the process we lose some of the predictive power of the original theories we leveraged. While at first glance, this may not seem to be an issue because the model is tested against the data, what we have done is effectively created a local fit. This means that we may have lost the ability to generate

the full range of potential scenarios that may result from a policy. This issue is described notionally in Figure 13.
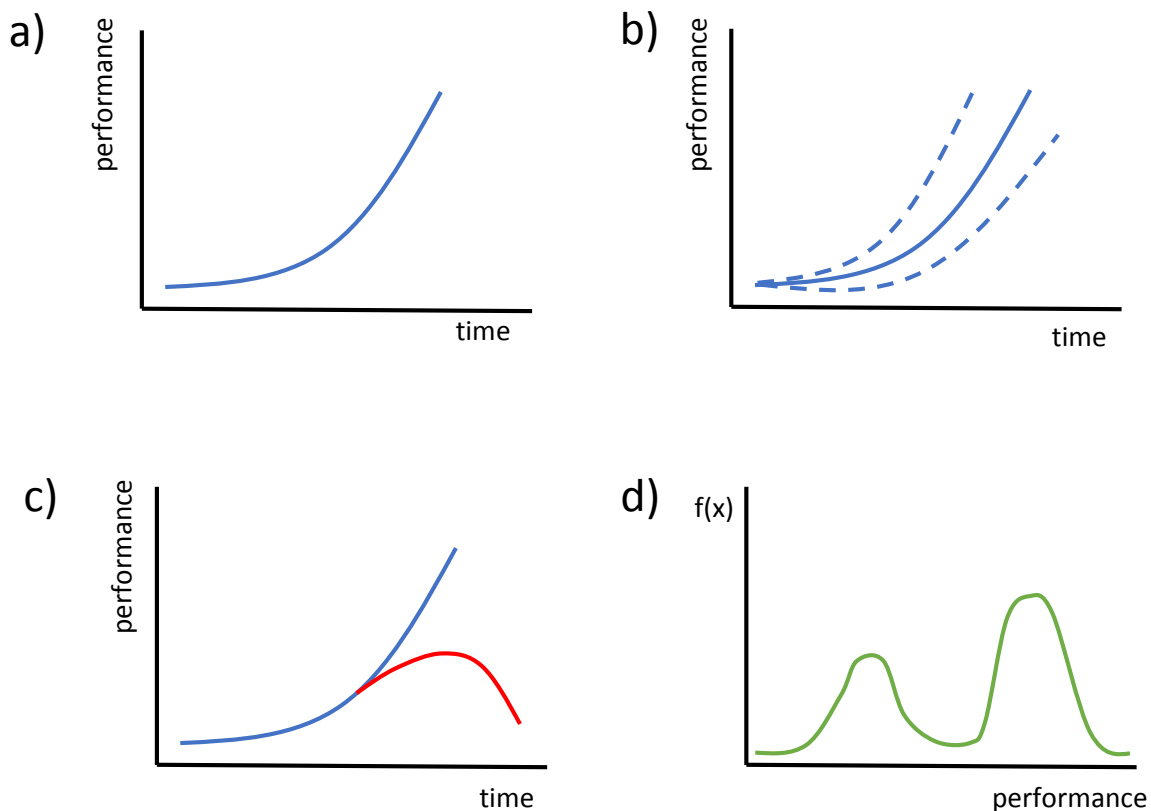
Figure 13 – a) When a model is developed and validated against historical data then used for prediction, it is equivalent to extrapolating a trend. b) Parametric sensitivity analysis or frequentist prediction intervals put upper and lower bounds on the trend but would not be able to detect a shift in the trend triggered by structural changes. c) Systematically introducing alternative structure to the model can generate alternative trends. d) The ideal output of such an analysis would be a multi-modal probably distribution of potential outcomes.

Once a composite model is built and evaluated against empirical data, we now have the ability to generate predictions (a). However, we know that there is uncertainty in the model so we perform sensitivity analysis or apply a more rigorous uncertainty quantification approach. The problem is that this typically done over the parameters of the model as there is a natural space to vary these over. This results in a distribution of possible outcomes represented by a prediction interval in Figure 13 (b). However due to the model development processes described in Figure 11 and Figure 12, some of the predictive power of the original theories is lost. We can think of it as some of the structure has been thrown out either through the partitioning or refactoring processes. Furthermore, there may have been alternative abstractions that could have applied to the original conceptual model, but for whatever reason, were not selected. This, too, is lost structure. If there were a way to reintroduce this discarded

structure, it may generate predictions that are very different from the ones produced by the built model (c).

Depending on the circumstances, these alternative trajectories may be assigned an extremely low probability under conventional sensitivity analysis. That is why when these trajectories do occur in real life they are "unexpected," "unintended," or "counterintuitive." What we would rather have is a more justifiable approach to developing model predictions by systematically introducing this lost structure. This would result in a more complete probability distribution of potential policy outcomes. Notionally, this could be viewed as recovering modes in the distribution that were lost as consequence of the model building process (d).

7.1.2 FACTORS FOR CONSIDERATION

If we would like to systematically explore variations in model structure to generate a spread of scenarios like those depicted in Figure 13, there are several factors that we must consider. First, when developing a composite model, we are not totally unconstrained in our selection of abstractions. For any policy (or design) problem there are typically a limited set of factors under our (or the policy maker's) control as well as particular set of consequences that we hope to achieve (or avoid). This naturally leads us to a limited set of control variables and response variables. These significantly constrain the model development process as any model built must provide a complete linkage from control variables to response variables. When the control variables and response variables lie in what are traditionally considered separate abstractions, this can be very challenging. Unfortunately, this is the usual case for an enterprise problem.

While not an explicit motivation for the core-peripheral approach developed during RT-138, in retrospect, this was probably the reason that the approach emerged. The linkage between the control variables and response variables necessary forms the core. If this linkage is not valid, then the entire modeling effort is useless. Once the core is established, variations in structure or higher order structure can be introduced to trigger "higher order" effects on the predictions of the core. These are the peripheral models. In essence, we are looking for factors that "disrupt" the control linkage.

However, reflection on both the literature review and the mathematical analysis on multi-scale ontologies suggests that there are probably several different cases that a modeler may encounter. Each case may need to be addressed in a different way. Here we lay out each of the cases we have identified, though we note additional cases may be identified through future work.

Case 1: Direction integration of peripheral models with core model

In this case, only state linkages exist between the core and peripheral models. As a result, peripheral models may be swapped in and out as needed. While this may happen due to "luck," the more likely situation is that the modeler refactored the conceptual model to remove

transition linkages between the core and peripheral models. In retrospect, this was the approach taken during the development of the counterfeit part intrusion model during RT-110 and RT-138.

Case 2: Separate peripheral models with handover to core

In this case, there are one-way transition linkages between the peripheral models and the core. This case is analogous to multi-fidelity modeling approaches. The peripheral models may be run first and then the resulting outputs can be handed over to the core model as alternative parameter values. The core model is then run second.

Case 3: Partitioning the state space

In this case, the two-way transition linkages cannot be eliminated through refactoring. Consequently, the only solution is to partition the state space and apply different abstractions to different portions of the state space. Here peripheral models are alternative representations of these portions of the state space. This is analogous to multi-scale modeling where the alternative models for each scale are switched in and out. The problem here is that potentially new empirical "handshake" algorithms may need to be developed for each combination of models.

While all three cases are important, for the approach developed in this report, we will focus on case 1 as it is the most tractable. However, it is expected that the developed approach is extendable to facilitate cases 2 and 3. It is likely that category theory will play a role in accomplishing this extension.

7.1.3 STEPS OF THE APPROACH

The systematic approach to developing an interoperable core-peripheral model is illustrated notionally in Figure 14. Essentially, this approach combines elements of both of the existing approaches presented above. Again we start with the conceptual model (a). This time, however, we identify the control and response variables, and identify the relevant paths between them. These paths are candidates for establishing the core model. At a minimum, the core model must include at least one path from control to response, but multiple may be included. Presumably, the core will include what are perceived to be the most "important" factors. In essence, this would be the "first order" representation of the system (b). This core is then represented using some combination of refactoring or partitioning to manage transition linkages and create an internally consistent model (c). The portions of the conceptual model that were omitted from the core are candidates to become peripheral models. These are refactored to eliminate transition linkages between them and the core. Note that there may be more than one valid formulation of each peripheral models, particularly when the peripheral models represent behavioral and social factors. Finally, mathematical and/or computational models are developed for the core and peripheral models (d).
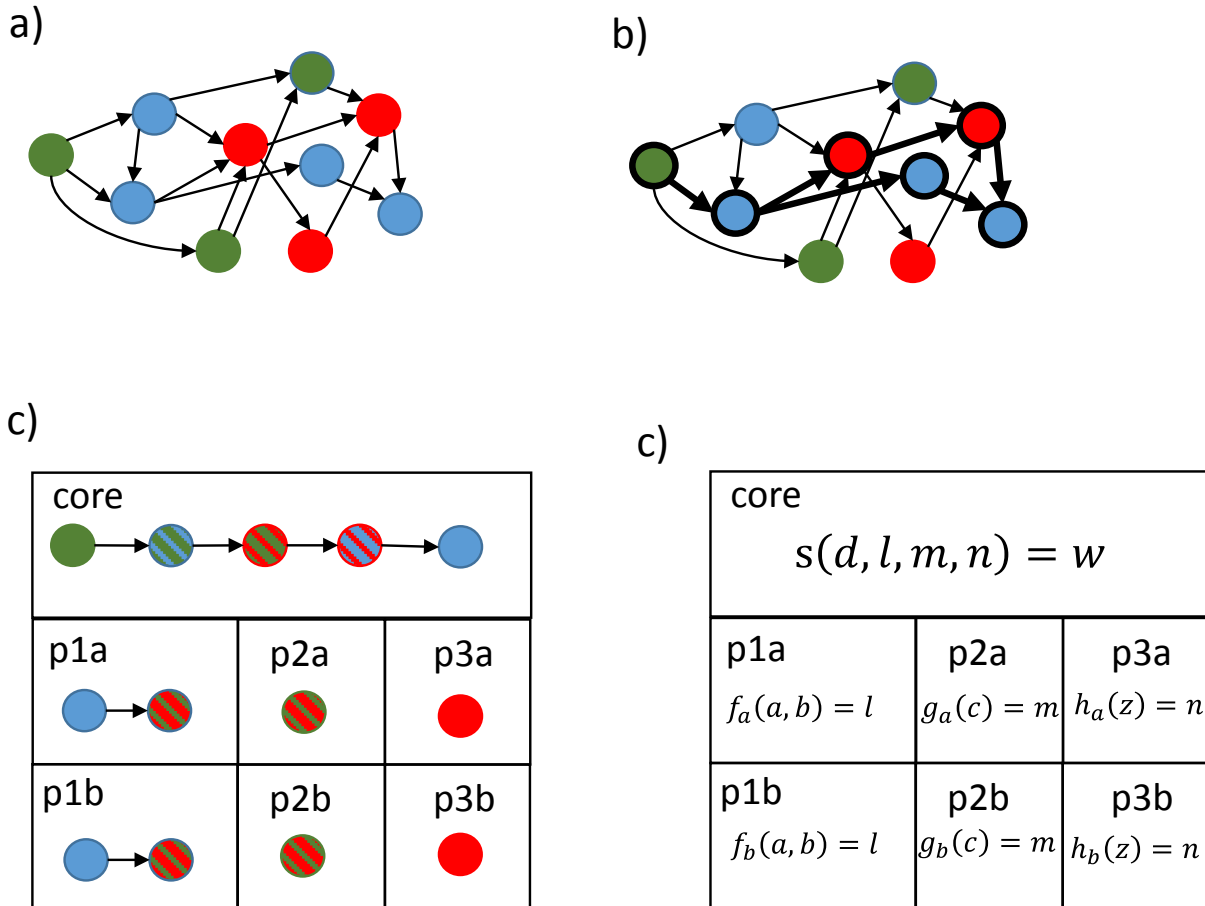
Figure 14 - Systematic Approach 2: a) Initial conceptualization of the system will likely involve mixtures of many factors and relationships from different absractions. **b)** The modeler identifies the control and response variables and identifies the most important chain of relationships between them. This constutes the core. **c)** Since the abstractions are not necessarily compatible, the modeler modifies the factors and relationships to create a conceptually consistent model consistent core model. Factors that are off the core paths are candidates for periperhal models. These are refactored to eliminate an transition linkages with the core. There may be more than one version of each peripheral model. **d)** Since there are now a set of mutually consistent conceptual models, they can be represented using consistent mathematical or computational models.

Since the transition linkages have been eliminated, the core model can be mixed and matched with the various peripheral models to generate alternative trajectories. Each combination would generate a different scenario. If probabilities are assessed for each combination of models, it becomes feasible to generate a probability distribution for the set of possible outcomes.

A few things to note:
- There is no guarantee that it will be possible to refactor the conceptual model such that there are no transition linkages among the core and peripheral models. As we noted above, we are focusing case 1 first. The presence of transition linkages would trigger either case 2 or 3. In principle, these can be accommodated, but will require extra steps.

- It is critically important to validate the core model. This serves as the baseline for the subsequent analysis. If it is not credible, then none of the results will be credible.

- The integration of one or more peripheral models into the core generates alternative predictions, but there is no guarantee that they are real. However, they do establish possibilities that could be further investigated or hedged.

- While one could probably perform a full factor analysis for a relatively small number of peripheral models, as a practical matter, there may be many possible combinations of peripheral models. This will be particularly true for peripheral models that represent complex phenomena such as behavioral and social factors. Consequently, there is a need for an approach to both identify potential model formulations as well as navigate through them in a reasonable way. This will be addressed in the next few sections.

7.1.4 VALIDATION

One obvious question about the above approach, is that of validation. What we propose is that validation efforts focus on core model. The reason being, as stated above, is that if the first order model is not credible, then the rest of the modeling effort is irrelevant. Thus, this model should undergo rigorous evaluation by subject matter experts and tests against data as appropriate.

Note that it is critical that the core model be validated in isolation from the peripheral model for two reasons. First, the core model represents, in a sense, business as usual while the peripheral models represent departures from business as usual. One cannot assess the impact of the departure if the model representing business as usual is miscalibrated. Second, peripheral models introduce additional degrees of freedom. Attempting to validate the combined model is essentially self-defeating as it increases data requirements for validation and confounds the very relationships we are attempting to tease out. In essence it devolves to the interpolation case described previously, which is exactly what we are trying to avoid.

As far as the peripheral models themselves, they should be structurally valid, meaning that they conform to known theory or data, but it is less important to validate them in isolation. Their role is to support the equivalent of "what if" analyses. So the question is not necessarily whether we know them to be representative of current or projected circumstances, but rather we want to know what will happen if we assume they are representative.

Once experiments are run by varying combinations of peripheral models with a validated core, there is a question of the validity of the predictions themselves. While this is somewhat dependent on the circumstances and the system being model, we may never know. There may be some circumstances where we can run an experiment or collect some additional data to test a prediction. However, when we are concerned with policy, we may be dealing with

counterfactuals. For instance, when a government chooses a particular macro-economic policy, we will never know what would have happened if they had chosen a different policy. In these cases, the various scenarios generated by this approach may be untestable. Subject matter experts may be able to eliminate some based on infeasibility, but the remainder should at least be considered as potential scenarios in the decision making process. These can feed strategy development much as scenario analysis is used in strategic planning today.

7.2 POTENTIAL DIRECTIONS FOR ORGANIZING MODELS FOR USE IN ENTERPRISE ANALYSIS

As discussed in Section 5.2, there are issues and challenges associated with formulating models from social theory. Given both the variety of different models and their associated ontologies, there is a question of how these should be captured and organized. Of interest is providing a means for capturing theory that contains some social phenomena that can both maintain the domain validity issues and "store" theory such that a conceptual model can be presented. Then the conceptual model can be "compressed" and assessed applying the modeling and simulation principles described in Section 6. The motivation here is to catalogue social theory validity in the appropriate model theory. Then observations in the enterprise system of interest would have a "place" in an enterprise model theory. The goal is an approach and schema for transforming these into a systematic approach. In this section, we consider the required identifications, relations, and 'higher-order' types. Next, we describe the problem up to ordinal theory and develop a systematic means for constructing categories as a working hypothesis. This provides useful encapsulations for social theoretic components and highlights categorical relationships as potential research domain. It is hoped that, when fully developed, this approach will present a useful framing to maintain consistency within social theory and provide a formal mechanism to guide practitioners and modelers when integrating social theories into their enterprise models. It should be emphasized that the following presented approach is just a tentative hypothesis intended to provide a starting point for investigation. Much additional research is required, and it is expected what is proposed here will evolve substantially.

7.2.1 SOCIAL CONSTRUCTS & NOMOLOGICAL NETWORK

Continuing from the social measure theory review in Section 5.2, one ends up with measures that provide functional mappings but only after sufficient definitional search. Ideas of how to provide appropriate 'objects' and their valid relationships (construct validity) were touched upon. There were two 'approaches' to the analysis (EFA and CFA) with the intent to get an available extendable representation (PCA). The crux of the analysis was considering the 'higher-orders' under the appropriate structural context which involved assessing more than just the internally available observations. This gave a causal description but these theoretic and model statements were not 'nice' in the deductive falsifiable sense. These descriptions while measurable were not (necessarily) identifiable, and if identifiable consciously, were not (necessarily) measurable. We reason here that this defines any theory constructs itself in some ordinal above the modellable compression.

We then showed that there were some implications where categorical structuring was applicable in some situations and similarly that people present categorical 'choicing' in the model theoretic sense. In sterile measurement conditions or by bounding the 'system of interest', these bounds provide identifiable decisions, measurables, and other model descriptions. But 'in the real world', we attend to a multitude of unbounded decisions in which individual and group choice induce orderings. Behavioral economics and social information theories argue that certain behavior localizes to a bias estimate (Tversky & Kahneman 1981), an ordering (Hayek 1945), and a choice (Arrow 1951) emerges without any individual being directive. These then might not be 'measurable' even if subjectively reported, or conversely, if it is reportable, it might not satisfy all possible descriptions. This to say that a particular universal descriptor may not be complete as a compression, a priori, and this by definition would have consequences 'unintended' by either the individual or a group policy response.

With this in mind, there is a unique perspective toward modeling when a component theory involves a domain of psychological or social science. There is not only the potential for yet 'unseen' effects with traditional observation, but there are potential reorderings in the algebra, and the representation of that algebra might diverge compared to the individual's 'mental model' structure. Even then there is a post-modernist perspective that under a language individuals 'bifurcate' and this adds a complexity under this 'intermittent' algebra (Susen 2015). This would be even less accessible than the previous as this extends the space under measurement (i.e. the individual has a measurable extension outside group setting that the individual is involved in). These distinctions make for dual considerations plus extensions within language all within any 'psycho-social' component. By argument, we propose that this points to a basis in typology and potential classes over model validity that are needed.

Since both the 'individual' and 'group' objects involved in a model can have differing associations under any instance, one involves an ordinal function in any multi-scale or multi-ontology modeling, and this directly influences how the objects operate influencing the 'appropriate' simulations. This opens the discussion to logics embedded within the 'post-modernist' tradition, but as a measure theory, these traditions have not been sufficiently defined. While we will touch on the notions, the engineering need is to translate the encountered discussion into an associated model theoretic framework if only to allow us to internalize the framework limits. Ideally any 'nice' engineering approach would try to objectify and reduce where possible or efficient, but these lack in topological constraint. Clearly, there is a need to identify where the models are limited and to develop associated guidance of their application. One would also want a pseudo-metric on the associated contribution to model risk; for example needed additional inductive assessments or potential consequences of an additional constraint. While these social theories are outside of the conventional systems engineering domain, the point is to make available of a variety of programs, logics, and representational objects available given by social scientific theories to enterprise modelers. However, this requires systematic attention. These 'human and social phenomena' are still describable using a language accessible to individuals and groups however 'soft' or self-referencing. At worst these are then higher-order language types that are used to describe over 'lower-order' objects, yet would still be a starting point for a hypothesis.

Because of this, typology around construct validity serves as a starting position for model theoretic descriptions. Over metric spaces, this has interesting logics and ontologies that are useful for systems methodology. For those objects that are externally definable, class association are described as employing a "pattern-matching logic" (Shadish et al 2001). As described by Shadish:

> *"The most common theory, each construct has multiple features, some of which are more central than others and so are called [more] 'prototypical'. To take a simple example, the prototypical features of a tree are that it is a tall, woody plant with a distinct main stem or trunk that lives for at least 3 years (a perennial). However, each of these attributes is associated with some degree of [uncertainty]. For instance, height and 'distinct' trunk distinguish trees from shrubs. But what some trees to shrubs [have these as ideals]. [So as described by human systems], no attributes that are foundational are foundational. Rather used a pattern-matching logic to decide whether a given instance sufficiently matches the prototypical features to warrant using the category label, [more importantly] given other available category labels."*

One can see where constructs can be argued from a stance over fuzzy logic. If one is trying to 'assign' a set item from a 'fuzzy' class of "tree", then one can use fuzzy logic for inference potential and assign set descriptions to profiles describing the 'fuzzy' "tree" form; e.g. normal curve around say x height to be tree. One would then need reliable observation or theory for the 'tree' prototype and even then relational statements between it and 'shrub'. For an enterprise, the need would be to assess the self-defined objects and the potential fuzzy classes for which these have relationship. But these 'theories' are then subject as Shadish notes that the class of "tree" itself is a fuzzy notion in the domain of the mind when we attempt to simulate it in the mental models. Now one could continue ad infinitum indexing fuzzy object relationships by making increasing order on probabilistic assignments to class, type, and object to converge a space (i.e. a Bayesian net framework). But then one asks what 'bounds', 'limits' or similar topos property show that the general openness is reasonably closable in an instanced context. This to show that an enterprise is left with the satisfiability problem at the universal even when an instanced situation is has a Bayesian solution. In mathematical model terms, the openness in its algebraic and topological uncertainty does not necessarily give generalizing categorical properties or convergent algorithmic properties.

This then becomes an epistemological problem of satisfiability over various mental models against the models of any 'technical' nature. Latent considerations dually approached itemized, algorithmic (i.e. set theoretic) responses by considering both analytic and algebraic objects as was seen. There were linear algebraic descriptions on the response profile in specific intelligences, and one then collects more generalized description in models from the inductive

support of fit statistics. Understandably then using statistics to measure first order responses is useful as they have definition over the natural measure space (i.e. itemized measure themselves), so it is not as if humans 'invalidate' the natural properties over this 'model order'. For instance, one measures a pilot over a flight model to measure pilot behavior, and involving a human mind does not invalidate the model setup as measuring a pilot response has strong validity when comparing this behavior under the 'flight model' constructed model. This may seem unnecessarily tautological, but this is what a 'natural limit' or 'boundary' gives us. If the pilot does not execute under certain constraints, it is likely that the plane will crash, and this gives us a universal to solve our 'ordering' problem. Additionally, this schemata is given a priori, so one can fall on reason even when supposing a large space in which behavior can operate.

Now consider extending the model and reusing theoretic descriptions and moving to a generalized theory. Now we must deduce the constructed boundaries, validate the abstractions used, and analyze whether these constructs relate to each other under our considered transformation. Within a 'local' model, the item descriptions are deduced themselves and used to induce up to a general description. When extending a model, it 'reuses' the base and analysis, and for parsimony, a modeler has to validate the description and boundary involved. This is not absent in other areas, but as noted, the 'psycho-social' space has means for 'exploding' the constructed bases as human are order generators (increasing deductive potentials) and language generators (increasing inductive potentials). The bigger problem is then the setting of these generalized abstractions in 'psycho-social' space and their validation. Considering the general domain then has 'tuples' with the deductive-inductive categorical bases (i.e. a 'valid' construction). As humans as a set object can insert themselves in varieties of constructs and spawn them, this becomes an increasing algebraic problem.

However, it is natural then to 'halt' our considerations under different contexts. When a pilot goes into health care, generally people consider this as a different category which we can 'project' what is needed by the health care 'dimension'. This 'drops' some considerations, but as pointed out, this compression just involves tracing the inference potential dropped. A pilot-healthcare metamodel is assumed to be universally intractable across society, but we can rationalize that we care about particular information thus making it tractable. It is then an economic decision to determine what is involved in this tradeoff. When this invalidates an internally assumed construct represented in our language, the models become complex under composition. This is because some information was lost to the formal system about the boundary limits. When this occurs, social science terms it 'dissonant' compared to a mental model domain.

The 'halting' is done usefully by inserting a 'state change' (or similar 'cut') with the established 'pilot' and 'civilian' behavior. This identifies an ordering on the model space based on the mental model choice. However, then one begins to divide the model space for an individual and then the class of 'pilot-civilian' unitary set. This can still be split by other transformations or by assessing a choice procedure. The point is then one tracks the 'cross-sectional' between individual actions in the system with the available class descriptions (both conscious and

potential latent descriptions). Tracking then involves the inductive base, unit individuals, and the unitary class independently as components for validation. These bases are not always parsimonious, so the model theory space grows. What latent variable theory then tried to notice is when this expansion did not happen thus implying an observable point (i.e. anti-entropic phenomena) that can be assigned to a unique 'human behavior'. More interesting is when people change internal 'states' either consciously or not which presents an encrypted latency. So then one has to do 'pattern matching' across the cross-sectional which diagonalizes the model space and characterizes intractability. Thus, it is not surprising that model composition with social and cognitive aspects is not well identified.

So considered from an engineering perspective, 'social theory' does not always provide stable unit descriptions. For example, a 'unit' in social science may not be as stable as a unit in the physical sciences like the Watt. Rather unit classes are available over a given domain from the available language across individuals. So having reliable factors for a 'pilot class' is not as available per se as knowing that a construct involves the 'pilot class' itself. This then gives the determinable dimensional change and inductive bases involved. Also note all of this without a reasonable basis for these 'states within pilot<->civilian' does not have symmetry to the mental models (i.e. the 'rational' human mind is not universally parsimonious to its own behavior). Nor is there symmetric measure that totally configures under this "state change"; e.g. providing a brain scan as a means for establishing symmetry still has an identification problem (and thus does not necessarily satisfy). This then implies that particular measures are embedded categorical notions that involve trades on scientific and model language.

This then defines our discussion to consider the 'construction problem' up to sufficient type validity and the language involved. The instanced algebraic description and the topological mapping(s) invoke a protean categorical analysis as a model accumulates types and spatial constructions respectively. It is our impression that enterprise modelers have encountered this for socio-technical systems, and this underlies the composition and consequence problems. The incorporation of SME impressions and 'multi-leveled' modeling has defendable intuition in this regard as it gives these 'higher orders' rational constructions. These methods (or instances on these methods) then must manage compression in reducing the model space sufficiently to not lose the aspects under consideration. The attention within social science modeling is symmetric in discussion as it manages the same attention. Then the suggestion involves using categories to organize socio-technical system modeling as it incorporates descriptions that are 'social theoretic' in nature.

This becomes more apparent as system modelers consider model composition across reciprocating functions from observation. If assessing an abstract idea of 'tree' is sufficiently difficult to satisfy, reciprocating up the idea of 'plant' is even more, and ordinally more difficult is the 'idea' of 'environmentalism'. This and other similar '-ilities' are within purview of systems engineering and are validated by theory only accessible by mental models. The range on enterprise modeling extends up to then an ordinal concept just for a particular social dimension. This helps define why objects are readily definable in social theory, but their modalities do not close under collection. The representation remains an open question within

social science as how to handle these systematic descriptions on behaviors. And thus the given system representation having difficulty is understandable. Section 5 described the large body of work behind this problem, but the concern here is how to centralize the descriptions. Ideally then there should be sufficiency to mirror system modeling in both its representation, simulation, and most importantly informational limits.

Pragmatically system modelers can take a page from social modeling practitioners. One has to fall back on some realism if only to have objects with which to model and usefully simulate to determine the extent of their validity. Then one actively searches classes for these objects, assesses their prototypical properties, and then successively types the developed bodies of theory. Concurrently these are validated against the observed itemized descriptions and mental model context through experimental design, higher order pattern matching, or causality as an ordering (Shadish et al 2001). There is a strong and growing body of knowledge that mirrors soft system theoretic development as these are creating conceptual, generalized theoretic compression.

An encountered idea that helps support our 'categorical mapping' claim toward enterprise modeling was embedded within the construct validity literature. Cronbach and Meehl (1950) have a classic paper where they consider the prototype theory as a 'nomological network'. This mirrors the graphical representation within latent variable theory where the open transformations are represented by network connections, but one would recognize their argument mathematically as an algebraic network with categorical relationships. They argue that these successive identifications in ordinal space creates a topological network for the underlying 'concrete' descriptions. Campbell and Fiske (1959) relate this description to a diagonalization process in a measurable space in which to assess these open relationships. There is then a formal stance that this identifies potential descriptions with increasing power in the "network of nomologies". The description here is that pattern symmetry implies congruence between algebraic categories. Categories are used in other areas, and the argument here is that the patterning over large-ordering devices (i.e. 'human' in all our capacity) involves constructs that have unique universals in validity under different instances. Campbell and Fiske present a Multi-trait, Multi-method matrix representation that enterprise engineers would appreciate. The effect is to gain increased power on cross-validation by successively rediagonalizing the space.

This then supports the conjecture that there are inter- and extra- model properties that determine the universal and multiversal validity respectively in sociotechnical systems. 'Constructs' define an ever cascading indeterminacy that is categorical in nature. Naturally one thinks to use category theory as a 'language' that could serve as tracing 'compression'. This does not solve it per se as in the end the goal is to provide objective output, but representing theory in categories would trace the 'higher-level' orders more clearly. For example, Rosen's categories do not eliminate complexity but rather one can identify the simplifying relationships easier. Cronbach and Meehl (1950) claim that this 'categorical compression' is needed and its potential (this author emphasis):

"With these statements of scientific methodology in mind, we return to the specific problem of construct validity as applied to psychological tests. The preceding guide rules should reassure the "toughminded," who fear that allowing construct validation opens the door to nonconfirmable test claims. The answer is that unless the network makes contact with observations, and exhibits explicit, public steps of inference, construct validation cannot be claimed. <u>An admissible psychological construct must be behavior-relevant (59, p. 15). For most tests intended to measure constructs, adequate criteria do not exist.</u> This being the case, any such tests have been left unvalidated, or a finespun network of rationalizations has been offered as if it were validation. <u>Rationalization is not construct validation.</u> One who claims that his test reflects a construct cannot maintain his claim in the face of recurrent negative results because these results show that his construct is too loosely defined to yield verifiable inferences.

<u>A rigorous (though perhaps probabilistic) chain of inference is required to establish a test as a measure of a construct.</u> To validate a claim that a test measures a construct, a nomological net surrounding the concept must exist. When a construct is fairly new, there may be few specifiable associations by which to pin down the concept. As research proceeds, the construct sends out roots in many directions, which attach it to more and more facts or other constructs. Thus the [social quanta] has more accepted properties than the [physical quanta]: numerical [properties imply] more than the second order factor space."

However given the intuition that categories are congruent in form to a 'nomological network' allows one to notate the 'definitiveness' on a construct network by assessing the "finespun network of rationalizations". So these "chains of inference" are then congruent to a particular 'universal functor' in which to then define a category. The potential benefit is that if so-called 'nomology logics' are available that these would inherit categorical theorems such that one can test these both ways: the numerical 'small category' from deduced observables and mental model 'large category' from induced bases. This then potentially guides the aspects to identifying unintended consequences as one would like to know how these 'large category' constructs insert into 'small category' system (various mental models potentially effect a system of interest) and how then 'small categories' might be constructed that are parsimonious to encountered 'large category' abstractions (identify the consequences from previous validated models).

These then imply via use of categories that algebraic properties must be matched ('commute' across all large and small involved). Otherwise there will be multiple types of 'model bifurcation error': invoking a system under unjustified mental construct, invoking a mental construct that does not present in the system, extending a system without symmetry in the

extension of the mental construct, and likewise extending a construct without parsimonious system model composition. These are then 'dissonance' issues between the observable world and the mental models. But system observation could be compressed to a 'large category', and these serve as a class-type language in which to simulate and compose measurable models to validate at instanced 'levels'. While this invokes the intractable 'algebraic problem', this allows more dimensionality on enterprise modeling that can be assessed. Information theory's ordinal numbering shows that some compression is irreducible, but also helps identify where programs are self-delimiting. Additionally, this seemed more 'natural' to the analysis observed in psychological and social sciences, so would be parsimonious in categorical language. For example the IQ theoretic statements defined and shown measures over the 'open set' space on a topology. Then by its theory the measure had difficulty extending over any 'closed set' space: item by item ordering and individual by individual ordering both of which have a denumerable setting. Where IQ was valid was over group orderings, it is conjectured that it is due to the openness invoked by the groups and opens the simulation space. However, this itself lets modelers know a priori that there is limited 'extendibility' in evaluating sub-group systems, so there is still 'information' in some fashion even if in its architecture.

7.2.2 CLASSES AND TYPES IN NOMOLOGIC MODEL THEORY

When attempting to build a nomologic network, one deals with multiple potential orderings embedded in a particular set-type-class grouping? So how does one compose a set ontology in parsimonious way? As Cronbach and Meehl (1950) noted, this does not make any set language always unsatisfiable as one can construct using increasing power setting, but then tracing these through the openness becomes increasingly difficult to get 'validate-able' descriptions in the system of interest. The open structures then involve complicatedness (given a setting is transfinite) and complex (given otherwise). Then the network representation is necessary to maintain the extent on proper orderings that are not immediately denumerable (implying a settable linguistic).

Ideally, there exists a definitive ordering constraint at some 'level' in the system or mental model. Provided that a modeler can use a higher ordering assumption (e.g. multi-leveling, 'ontological' classes, and other set ordering), he or she can insert a 'construction' that then needs to be justified, identified and validated. Otherwise, for computability, it must be embedded in a real measurable space which can compress to dimensional patterning, but then the potentially useful orderings for system simulation become hidden (i.e. embedded in the ordinal sets). Again, if there is a transfinite order, there is potential higher ordering that can be set by aligning mental model descriptions to a type hierarchy and the resulting language which a system can be based. But from work on the continuum hypothesis, this is not 'accessible' purely by denumerable systems (i.e. using itemized objects). Then in the spirit of information theory, one would like to compress it to a transfinite type hierarchy maintaining the categorical 'construct key' for the formal system. Then under composition, a modeler would like to assess the compression to provide a fuller theory on the higher-order types and maintain a spatial

mapping like a network for these nomologies, which as assessed in Section 6 was the intuition on conceptual models.

The fundamental transformations in Section 6 were 'reversing' by giving a denumerable basis and assessing using open sets giving an analytic basis. As we compose these, the types make for increasing abstraction. In social environments, this can lead to non-symmetric representation without clear mental models or convergent public choice. Note then this does not even make an instanced compression per se 'wrong' as the social group might have sets and orderings dissonant to 'their' itemization. For example different financial system models can be 'dissonant' to each other depending on the underlying stance such as derivative and value-based. These can show divergence from each other, but we do not think these definitively mean these are 'wrong' purely against each other. One can observe that derivative captures the 'openness' induced by 'hedging' and conversely 'value' on the open 'utility'. So then purely rationalizing over the large abstractions is not sufficiently, universally valid under its own system. These are simply compressions which require validation to their quotient, the composition operant has a valid isomorphism, and their 'large categories' stay homeomorphic to the system of interest. The point is this 'strong' validation requires an intense power setting to achieve otherwise there is limited inference from epistemic validity notions under just the formal system or mental models independently.

As a validation, the system of interest is either tautological in its reality, under experimental designs or *in situ* (under defined, normalized context). This means any extensions have to have proper unions in their set measures and then at (some level) provide a transfinite ordering to set its presented output. The financial engineering literature serves as a prime example as the theory has inescapable realities based on categorical properties inherent in utility theory, Brownian motion, contractual agent responses, etc. These classes might not be 'true' in totality (presumably not all human constructs are hedging and pricing behavior), but serves as an 'ideal' compression as there is then a proper, traceable categorical class on all behavioral quotients. This then allows greater setting with which to itemize, and then yields more powerful observation as there is a clear class ordering and known valid transformations implied by its nomology. One can use a transfinite inductive procedure to support model-theory constructions and again show traceability and satisfiability to the system of interest "as categorical defined". If the settings prove proper, then our nomologic network becomes a proto-type algebra, and if properness is not available, then there are clear modal statements with which to test further.

In the meantime, one needs to trace the complexity such that the variety on ordering, class, and types can be 'stored' and 'searched' in an efficient manner. The search is to find potential transfinite compression allowing universal closure, and this while 'storing' spaces provided by constructs previously identified. The theorems over categories and extensions serve these purposes given the topologic algebra being invoked by these compression types. Then one considers how these model and theory statements are to be 'stored' in a settable manner. There is an underlying 'inconsistency' as how does one set an unsettable phenomena, but one could number by the ordinals themselves as a means for delimiting the constructs themselves

when assessing the mental models (rational hypotheses on the "surrounding network" in a space). Below then are then identified modal properties implied by two identified axiomatic set theories.

Tiles presents a good assessment and representation to visit regarding the constructability on these sets (Tiles 2004). The investigations into axiomatic logics using Cantor's and Hilbert's programs gave strong power to abstractly construct settings and trace transfinite orders respectively. The centrality was not accounting for the wealth of 'settable things' but rather the growing power set on their potential orderings. There is shared intuition here as given the self-creating and spontaneous orderings in social systems one is likewise not as concerned by the set items but rather the wealth on transformative orderings. Godel's theorems on satisfiability then seem intuitive that the 'construction procedure' by Zermelo et al does not allow for 'accessing' these increasingly open ordinals; again not impossible but 'inconsistent' internally to the models set in this way. So this colloquially constructs a model space that cannot have a single universal setting to switch between a mental model and the world as it is ("rationalization is not construct validation"). Using this as an analogy to the ordering within a social system, it should present the difficulty in getting to a sufficient 'social theory' using purely denumerable, set statements *and* conversely ordinals themselves do not provide statements that are 'validate-able' in a formal (denumerable) system.

The intuitive consequence to using these together is the ability to capture computational systems and patterning independently. Then, as discussed, one can program in functional transformations on the models under a bounded domain. This is complex and thanks to impossibility we lose certainty in our transfinite setting on our control system. However, in social measure theory, there is accessible measure here which implies some constraint on the transfinite, social space. One final appeal, their approach has been to define through small and large categories the extent to which these can be defined constructively or openly respectively. Interesting results in category theory are under defined universal relationships ('functors') using that can extend the small and large categories ('Kan extension') which under the social theory would be synonymous with the "spun network" (i.e. extension) of 'constructs' (sub-universal functors). As these are algebraically constructed, this allows for transfinite constructions under sufficient identification over some meta-properties. Something systems engineering would like to bring to these 'socio-technical' spaces!

Consequently, the goal is 'two-sided' as any analysis yields loading open ordinal sets and 'proper'-ness at some spatial location. This then seems natural to identify systems up to morphism to some available small category that preserves the large categories involved. This allows a clear procedure that separates the denumerable expectation from the open construct being claimed. This is not new in systems engineering as agent based modeling involves social network theory implemented often using a topology. This is usually done by 'constructing' the openness as 'social relationship', a large category, while seeking to present denumerable agent responses, captured in a sufficiently small category, against each other. Then one constructs smaller categories out of an observable large pattern, and for a general (denumerable) theory in this area, one would need to show a definable transfinite order up these 'categorical layers'.

What is needed is to extend or simulate these categories showing that the social space is then valid across these modalities in a system of interest.

7.2.3 TRANSFINITE IDEAL CATEGORIES

A systems engineer would then like to develop these large and small categories to identify either a space or language respectively. One step would be to identify a basis and unit respectively, but by definition (or rather by impossibility theorem), these are not (sufficiently, completely) available. So then rationalizing via categories these to an 'ideal' construction is needed to fit a particular purpose. This ideal would then ideally be developed such that all large categories are an ordering that are homeomorphic, large to small category transformation are homomorphic, and small categories have proper classing (implying a set ordering) thus giving an executable architecture. While this implies choice ordering itself, which may by extension might be moving the problem, the intent is to take the intuitive form on Turing's logical program (Appel 2014) but applied to functor satisfiability rather than denumerable setting.

The page taken from Turing is to justify an algebraic approach rather than trying to pose proper orderings. His was an attempt at resolving Godel's paradox by defining ordinal logic such that it bounded the space that gave numerical construction allowing valid replication (his concern was mechanical replication). Similarly one can ask by analogy, how does one transfinitely order a categorical hierarchy in a language such as UML/SysML type-class hierarchy allowing valid replication by an open, 'social' system? If this has a bijection, then the open system can naturally output in this language without loss; so this 'ideal model language' can both express and capture theory. As UML/SysML has background in specifying formal systems, the opposite domain to formal systems (i.e. the social system) is not parsimonious, so then pure compression by a single language does not universally satisfy a particular conceptual network. Humans as ordering devices show more than a single categorical language, so the conjecture is that a single language is not even stable. As latent variables defend the stance that psycho-social systems have ordinal modular properties, the need is to define the modules up to large categorical constructs rather than the small categorical type module. So then engineers should be motivated to identify an open language rather than a single set linguistic to provide a base for formal 'socio-technical' systems.

Since this is an idealized discussion, some justificatoin is needed. Appeals will involve classic results in logic, set theory, and extension to categories, and then these are used to conjecture a hypothesis on an 'ideal language' for constructs implied by the surrounding discussions. These should not be taken as sufficient from theorem (as this is an intuitive construction) nor in theory (as this is a schematic impression over general latent variables). The appeals will stick to the axiomatic systems in Zermelo-Frankel+Choice set theory (ZFC) and those that allow 'spawning' of classes at open ordinals in VonNeumann-Godels-Bernays set theory (NGB). These matched with available structural transformation relationships implied by overlaying category theory allow for enough ordinal space concerning the review encountered.

Tiles provides a descriptive diagram showing the intuitively constructed space. Using recursion, one covers ordinals growing a denumerable model. Working from agents as ordering functions, this is necessary as this would be an object at some ordinal greater than the zeroth ordinal if their behavior is to be captured. The increasing space allows for greater 'ordinal combinatorics' that can be numbered by omega:
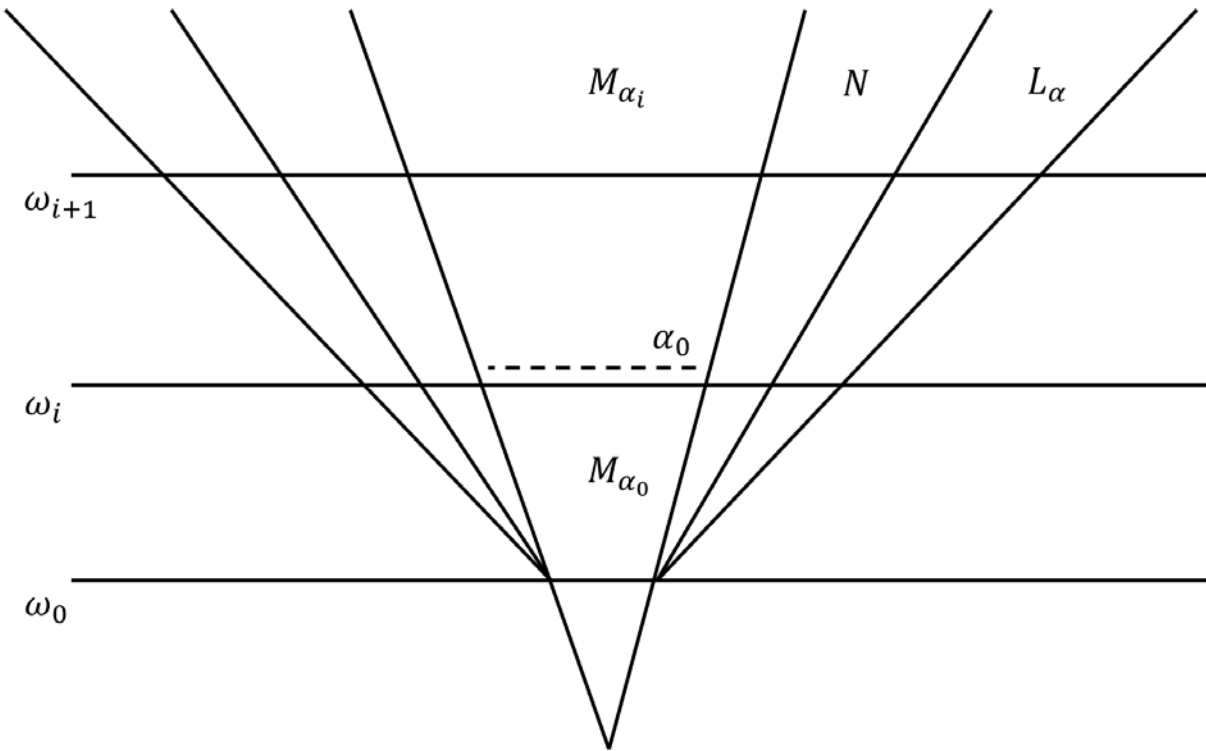
Figure 15 – Constructible Hierarchy (adapted from Tiles 2004)

A 'constructible theory' is then defined by traditional ZFC construction on a 'model' defined over some 'proofing system' which serves to provide which elements are valid under previous ordinal. Then a model at an 'alpha-level' has 'minimal model' that is strictly consistent within ZFC. That space which represents those 'constructible' statements which are potentially independent from the minimal model which can insert a function in the 'proofing system' that is given from outside analysis (i.e. a 'forcing' function). The 'axiom of constructability' seems a natural forcing as assessed from the mereologic validity encountered in the LVT conceptual review. Here the 'well-founded sets' are defined by a VonNeumann universe allowing those statements constructible in a transfinite hierarchy. Finally 'cumulative limit' defines the additional proper classes that (potentially) exist which are not 'nicely constructible', hence suffer indeterminate construct validity (e.g. construct fallacies that needed increasing diagonalization) in our system. The choice on NGB for this 'space' allows many of these statements to be specified on their own potentially independently of the formal ZFC model. It then fits the ideal that it has representation in a large category and available complex transformations therein (Muller 2001).

$$T_i^* = \{M_{\alpha_i}, P_\omega\} \qquad \text{- 'theory at aleph'}$$

$$M_{\alpha_i} = M_{\alpha_{i-1}} \cup P_\omega(M_{\alpha_{i-1}}) \qquad \text{- 'model at aleph'}$$

$$N_\alpha = \omega_i \cup \{a\} = L_\alpha(a) = \bigcup_{\beta < \alpha} N_\beta \qquad \text{- 'constructible', P with forcing, such that V = L}$$

$$L_\alpha \quad \text{- 'cumulative limit', such that V /= L} \qquad\qquad V \quad \text{- 'VonNeumann Hierarchy'}$$

Figure 16 – Hierarchy Settings (adapted from Tiles 2004)

The conjecture is this provides a nice capture on the nomological network within construct validity as defining NGB classes around the constructability allows the open mereology observed in psycho-social measure. This allows the 'model typing' that is needed for "testable rationalization" within a formal ZFC framework as there is the shared, nicely termed 'constructible universe'. Since 'unintended consequences' were self-referencing definitions on the constructability, this framework is symmetric and synonymous given the inconsistency in NGB allowing universal classes. There are then large categorical properties that can be loaded as ZFC has been shown to have an interface to topologically concerned modal logics; Morse-Kelly might be of interest from the topological analysis in 'social' and 'conscious' portions of theory (Kelley 1975). Then computational methods would be available given enough identification on these class compressions such that ZFC representation allows entrance on recent computational social science methods (Conte et al 2012). The implied hierarchical nature also mirrors the prototypical approaches in complex, post-modern classification approaches (Harvey & Reed 1996).

Specific 'niceties' on this interactive language allows those observations that as Gödel notes "is either too big for a machine or too small to be encapsulated by all of math" in some notational fashion. The set theoretic categories are then not a 'solution in itself' as these two are 'inconsistent,' but rather a powerful enough language which to represent abstractions. Then architecture in this manner would have natural 'modal types':

Captured Encapsulation	Modality of the Model	Set Theoretic Usage	Provides
Technical Aspects	V equivalent to L	ZFC independent	Current SE technical aspects
Interface	V homomorphic to L	ZFC with closed NGB	Composition under bounds
Interaction	V homeomorphic to L	ZFC with open NGB	Open interaction over construct
Socio-technical	V under L open limit	NGB under Topos	Open class relationships invoked under a constructed nomology

The later may be unnecessary if this 'social construct' is transfinitely settable in situ; e.g. classical economics shows consistency in certain contexts. This is shown by having a 'V-technical quotient' that provides a clear order in which to load a technical system. This presents a natural transformation that allows a VonNeumann-Morgenstern ordering to have strong epistemic validity given the proper classes are involved.

The dialectic implied by ZFC & NGB inconsistencies then could represent the post-modern difficulties with social science, and why behavioral insertion in economics have had difficulties. This is because capturing L as an independent(ly choiced) object is a difficulty but identified as needed within the studies. In other sciences, this is less trivial as the hypothesis method lets us infer 'L-language limit' and find the supporting evidence for the 'N-constructed universe' more straightforwardly (although in social science the N-'universe' is more accessible). Then one can define 'M-model' up to known 'N-universe', and this leverageable theory is 'nicely computable' as it is congruent to ZFC set theory. Yet when studying and imposing 'L-language limit' over a language generator something we hope is a given 'human nature', this appears as human 'adapting' that this breaks its assumed limits in an instanced theory. This implies that unintended consequences are a result from a formal systems language choice! This encapsulates the classic study problems such as self-fulfilling prophecies as being defined by this 'L-language' being extended and injected on 'N-universe' which would appear under measure as circular observations. Then the language device humans as a 'L(N)-language function' needs more ordinal space to be sufficiently covered. A 'L*-recursed language' could be constructed within NGB and then assessed for how symmetric this is to the current ZFC model. This 'dissonance' pseudo-measure could show the 'higher-order' phenomena in the NGB model. But the independent-ness between the two representations does not necessarily demand a formal system as public choice may determine this; e.g. engineers would not want to change entire aerospace development models instantaneously just because people imagined an unvalidated mental model for planes. This is then just a recursion on the cumulative potential in the population mental models which might be ultimately 'incomplete' in any well-formed 'N-universe' at ordinal level. But as human can carry on well enough without being well-formed in their mental models, this is then just independently 'dissonant' and requires additional steps to establish either's validity.

There could be new constructions by trying to develop both system models in both ZFC and NGB settings. This then allows a 'soft' ordering in our choice defining the epistemology with ZFC and ontology with NGB as one progresses in small and large category respectively. This can be assessed in social measure theory as the EFA + CFA => PCA seemed to imply categorical extendibility. Even more interesting, this might not be a problem as one could constrain the L* in NGB via a topological limit L*->L (ie pattern or topos) under some higher-order procedure. This would set the classes in NGB and be transfinitely bounded in ZFC giving a constructible metric framework up to an ordinal assignment. The categorical and topological papers implied this either by intent or by the underlying abstract mathematical construction. This might be (efficiently) incomputable by man or machine, but 'constructible' in the model theoretic sense such that socio-technical systems can have transfinite extensions despite technical constraints in any instance. Yet this would still be indexed dually by 'tuples' over the effective 'aleph-

classes' consumed in NGB before getting to 'nicely' modellable ZFC which is the central to the point to construct validity issues.

Then finding the uniqueness over NGB 'construct classes' is the inescapable epistemological solution(s). There is typing over 'construct categories' by their ordinal numbering in a 'nomology network'. While neurology or other biological extensions can 'build up' classes under NGB as well (hence the potential relevance and symmetry on these models and measures), this is only under such that N with the inference potential N-'morphic'->(L, L*) (i.e. there is a shared construct language). Now this can converge by adding analogies, but one must use a 'two-sidedness': validate a defined N-structure, observe changes in N, and monitor the adjoint under an ordered extension. This is covered by: ZFC for the instanced hypothetical validity, NGB which could assess whether classes converge & closes on a construct, and their relationship shows this 'strong' epistemic validity. If this is identified up to an ideal 'order-preserving isomorphism', then one has a full quotient for a V-technical space allowing a set system language to be used ubiquitously.

This seems the entrance to the Rosen categories in measure theory as one deals with these class constructions, but needs categorical relations in its meters within the 'well-constructed' system. In human inference, the importance seems reversed as possible classes outpace everything in which case the Rosen categories can be an easier compression on 'measures of interest'. This appears to one used to ZF(C) as terribly invoking class changes (likely why social theory and construct validity can appear to overly dismiss physical evidence), but under NGB, these can be well founded with hypotheses on their logical ability to split questions. In formal representative theory under denumerable sets (e.g. Newton's *Three* Laws), this starts to become a questionable intuitive approach over purely social enterprises as this leads to an overly constrained enterprise. This then conjectures possible trading on the class changes, and could use NGB classes previously identified to construct a [system, metric] pair to assess. This could give better assessment on operationalizing more 'general theory': Psychoanalytic, Gestalt, Psychodynamic, and the broad range on 'schools of thought'.

Finally, we consider the 'spawning' potential involved in the categorical extension. Economics has found interesting extensions in biology, physics, engineering, and social behavior. This is likely because if one has an ordered relationship mirroring a VonNeumann-Morgenstern utility space this provides a numerical basis on 'tradeable objects'. This could be used in categories to define over 'utility domain' that fits an 'economics category' as a construct. These are constructible in ZFC as these define a VonNeumann universe ordered by 'economic constraint' functor that could be applied over any ZFC-'model objects' under NGB-'utility class'. Given a defined pattern between NGB->ZFC, this intermediate category could be extended over several varieties that humans are involved under different orderings; applying economic games as ordering different 'levels' in a system. This also implies the wealth of economics less as a universal truth, but rather a regular pattern with which humans categorize so could provide extensions for behavioral economic encapsulation. Presumably in a formalized language, this could hope to find similar categories that relate a broad range of behaviors by assessing generalized theorem with different systematic bases. Then this would be defined by having

repeatable class compression with a denumerable basis whenever valid by transferring the class pattern.

The goal then is to provide a means for formally expressing theory such that is contains both the valid results (i.e. logics) but more importantly ability to mirror the appearance of 'unintended-ness' in the results. By invoking both ZFC and NGB axiomatic sets, this allows more descriptive power although not always a clear programmatic instance. Investigating how this systematic setup appears is at the heart of information theory in complex systems. The core observation is on replicating inconsistencies such that the logical setting internalizes but also gives resolution with a particular choice or proofing system. What would be interesting for systems engineering is the extent to how different independent axiomatic systems might be applied. For this case, this allows initially this 'separation' effect between observable models (ZFC) and human constructible models (NGB) and forces their interaction in a way that replicates the validity concerns in social measures. Categories are then useful as a means for maintaining order internally and communicating the systems to each other. It is natural then in category theory to use small categories to show ZFC, large categories for NGB, and identify functors that provide a map from objects in one to appropriate epistemology in the other.

Category's underlying representation in graphs allows the use by commutative diagrams. This also might transfer to patterning potential in human mental models as (Trochim & Linton 1986) shows an example of measuring graphical patterning. These in combination might allow measuring human patterns which can then be used as a (semi-)automata from ordinal observations from potential latent profiles. The graphical representation would have databasing potential for itself representation, and as again (Spivak & Kent 2012) has shown, there is a direct relational databasing output possible from sufficiently define categories. This would have the potential, given sufficient definition, to aid in decision making and visual aiding. The algebraic underpinning could also serve to 'solve' social systems in a more abstract manner as at any ordinal level any investigation could output to the closest "social norm" (Nyborg et al 2016) identified by the 'closest large category'.

Then begs the question as to how to create an ordinal topology sufficient for this space and how one 'loads' the database to maintain the objects across it (none of which is a small feat). Using our diagram from Tiles, we would 'copy' the image of the ordinal space such that choice ordering could be placed on the classed 'left-side' and choice ordered object model set on the 'right-side'. Then one would look for a functor or morphism that preserves the aspect(s) of the construct that one cares about: the invoked class ordering to the available ordering. This then allows a triple such that a construct is defined by its topos organization, functor, and itemized set.

The continuum hypothesis allows ZFC to reach a defined ordinal from power setting up to a particular aleph space (i.e. a 'bottom-up' architecture construction). Conversely class ordering can provide decomposition rules (e.g. 'top-down' functional architecture) allows for increasingly powerful NGB spatial identification. These ideally are identified up to an isomorphism for any intermediate ordinal space which would yield a 'nice', 'computable' theory

for any social construct. Likely this is not guaranteed, so one might identify weaker morphisms which still provides a 'usable', compressed theory. However each gives encapsulated objects which to have reducible relations in the category of sets with algebraic functions which can be simulated. This could yield (semi-)'nice' sets of theory which would have propositions in both 'technical' and 'social' space. These would still be complex but one could 'trace' observations by their 'n-tuples' of categorical choices. Then with any settable proper classes, one can again use Turing logical architecture against the modeling language themselves. Loading a generative automata from a sufficiently defined self-limited language (UML/SysML), and more importantly modulate it so that it knowingly halts when no longer in its construct domain!

The hypothesis is that this dual representational has power described above for 'socio-technical' systems. As a short patterning we show this over three arbitrary levels in a model architecture (Figure 17) as a first conjecture as to cover the purely algebraic typing at level (i-1), purely topologic typing at level (i+1), and the potential mixture modeling at level (i):
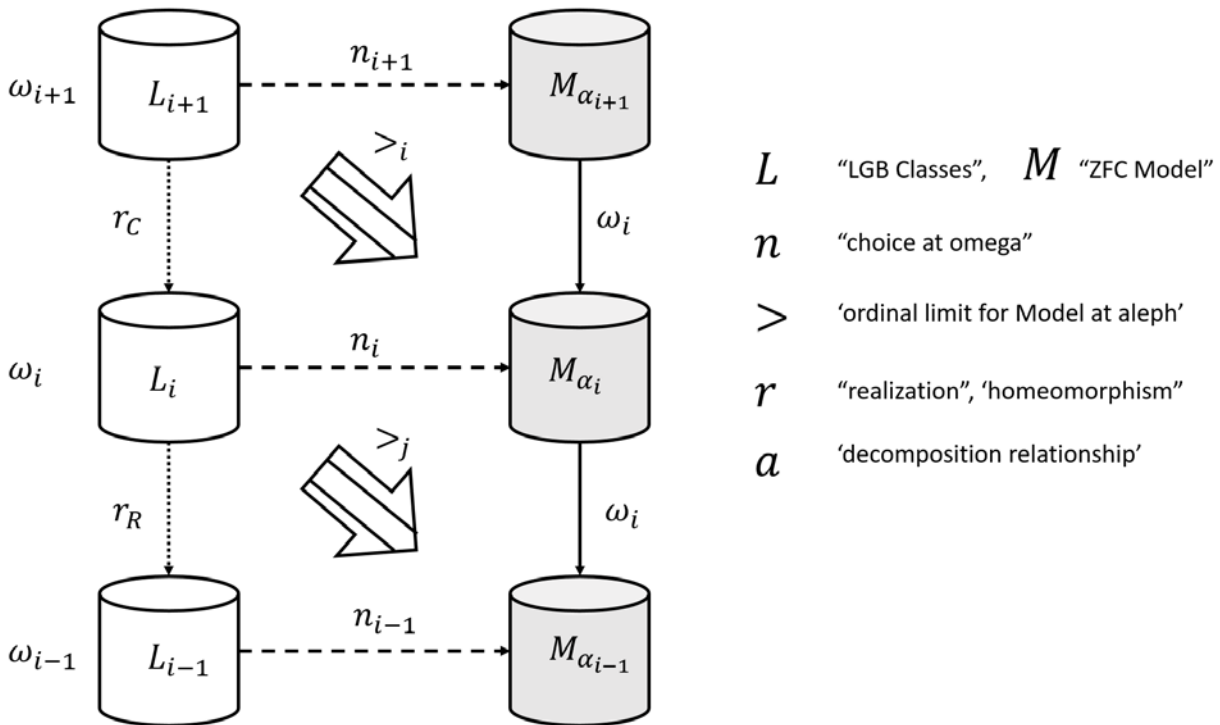
Figure 17 – Hypothesized dual representation

This yields a type hierarchy by conjecture over the constructability on the sets. These constructions as mereologics would then define a ordering for the system which could be assessed by simulating statistical social measures. This would also imply an 'ordinal confidence' as one 'moves up' the hierarchy which would allow a quasi-quotient metric for the constructs (i.e. the more mereologic specification, the more potential construct validity issues invoked). Likewise shaping statements such as '-ilities' specification could be represented by their class construction assessed in variety of instances that are validated as representative: by continuously assessing set SME statements, validated public choice ordering, and observing latent profiles in action. Given a sufficiently large library, then one could identify distancing

over the class compressions from various sources then useful abstraction in aspects in socio-technical systems. For example it would be useful to assess maintainability as a defined modellable metric (ZFC), assess that metrics serve as useful measure (SME/public assessment), this remains an ordered scheme (NGB), and searching additional schematic notions to define appropriate 'ontology' for an implementing architecture (choicing a M-'model hierarchy'). This could be specified in various orders via model assignment {a}, open set decomposition (r), and specification at ordinal level <n>. Hopefully this could serve as an ordered trace on any systems modeling procedure specified by constraint type, ordinality, and construct domain.

The hope is that this serves as a relatively simple category to type organize the socio-technical language but more importantly identify and cross-validate categories. As Gödel et al were concerned with intuitional organization, this might even prove to assist in transmitting better discourse on these open, intuitional aspects in enterprises. If the more open and dissonant aspects can be formed into a similar language, this might also aid in being a (semi-)automatic typing itself by again naturally incorporating both modellable and inherently inconsistent aspects. As set theory has been well realized in model management and activities in system engineering, categories then might also prove to assist in translating open aspects in socio-technical systematic programs.

7.2.4   DISCUSSION AND NEXT STEPS

As was discussed, involvement of social theory brings with it several abstractions that have to be negotiated. While there are clear physical objects involved, measuring, compressing and extending theory then involves aspects which are not physically instantiated. People's ability to order and generate language are underlying reasons for these difficulties. This has prompted social science to involve additional aspects in their studies, and these modalities are different from traditional technical ones. However this does mean that when involving a space which covers social scientific areas that it must inherit these modalities, and from analysis on the modalities, these become a complex system.

The theory encapsulation and the associated modeling involved must be able to deal with ordinals from human activity and abstraction due to language dynamics. These aspects do not immediately invalidate any model, but adds dimensions to its satisfiability and validity. While rationalization helps in this regard, there are potential inconsistencies in substituting rationalization with analysis and analyzing over a centralizing rationale. This involves any system self-analyzing its own inconsistencies and monitoring the ordinals induced, and this requires constructing a complete system against any context to be able to be validated against other 'constructions'. The review in social theory is that while the expanse becomes difficult there is plenty of constructible observables to use.

Identification of a system over ordinals and open linguistics as needed in this regard. The theorems in abstract mathematics gives a formal representation for these organizations of constructs. These mathematical abstractions and modalities can be identified up to the notion

of a 'nomological network' that underlies latent variable theory and other social theory. This should allow a presentation of 'constructs' that help give an abstract modularity within enterprises. The challenge then is maintaining a representational language for a system powerful enough to capture the formal abstractions involved. Apparent in social theory is the varied use over deductive and inductive procedures which then require an increasing program to incorporate the phenomena involved. The modalities in axiomatic sets and homotopic types within category theory allows means for these compressions.

A system with ordinal constructs then could be identified by small category representation, large category extensions, and tracing via transformations therein. The presentation did this with ZFC axiomatic set for the small categories and NGB axiomatic set for the large categories. Then the tracing exchange was around the instanced architecture (i.e. common transfinite hierarchy), and the extensions could be made for model composition around a 'construct' (i.e. a set large category). This allows one the freedom to be able to represent a multitude of potential languages across various orderings, but allows some abstract spacing as these must be noted with their categories, morphisms, and ordinal numbering involved. Any systems surrounded by context, constraint, and formality could then use a Turing (-like) logical program to develop any instanced enterprise system.

To investigate this system going forward will involve a broad and interdisciplinary aspects that are traditional to systems engineering. To simplify the discussion, the three aspects of the system serve as good initial types. The small category considerations are scripted as traditional modeling efforts so is a natural setting. The large category considerations surround current social science efforts as one imagines the involvement in open categories will require this in the study, and again the impression is the logic in the social sciences mirrors this. This then gives colloquial categories for 'technical' and 'social' respectively. Then system engineering efforts could be placed in investigating the research in those morphisms that serve applications. And of course, underlying all of this will be the abstraction language undergirding this from the mathematical sciences. This likely would involve a tripartite effort in case creation with a science investigating the implications of maintaining the inconsistent aspects in the dynamics on the ordinal placements.

As an initial area for theorem discussion, Arrow's classic inconsistency theorem provides a good candidate as it involves a 'linguistic limit' in the organization of decision making. Decision theory itself is an important discipline in enterprise systems and provides a common thread. The inconsistency surrounding decision and voting systems provides a large category with limit, and the extensions that have been developed provide smaller categorical 'transfer'. Likewise its ability to form another general construction in general equilibrium theory would provide another 'pattern' categorically. A categorical review on the model management aspects in these areas might provide insight in patterns in these ordinal 'public choice' constructs. The basis in theorem and rational models would provide examples of viable extensions as since has identified tractable subcategories from Arrow's original system (Reny 2001).

Conversely another area for the analysis models might be health systems as behavioral health is a complexity aspect in this area (Rouse 2008). A significant portion on the latent variable theory involved health behavior, and areas of community health immediately involve social psychological aspects. This creates a wealth of ordinal aspects with a technical underpinning (i.e. chemical, biological, and economic aspects in healthcare). This has been an important area for systems and enterprise engineering, and would by argument involve several categorical theoretic problems. Another similar area for analysis might be financial systems as econometrics and stochastic analysis provide categorically different measure theory set-ups. So then showing the spacing aspects in ordinals as a potential means for splitting the aspects over these measure theory might provide clear rational deduction on the descriptive power.

Overall there were many aspects found in research and enterprise activities. The important question is does the construct language appear this way under our rationalization or is this an actual underlying encapsulation? It would be pertinent to assess compression schemes involving language in a progressive manner to use the time and dynamics as an extra dimension for validation. This is a heuristic in social theory and likely then an important aspect herein. Additionally there is likely a multitude of existing modeling threads for category theory to encapsulate, so there is no immediate need to assess actual systems before investigating its possibility. This can be assessed by organizing system architectures and description aids via these categorical notions and induce the various valid aspects. Then having provided the 'there exists' portion can begin to inject in systems to assess how this works as a universal capture. The wealth in documentation, case examples, models, and theory should provide many places to start.

Lastly for the aspects involving enterprise and socio-technical systems, this leaves a wealth of space in which to investigate but also questions of which to be mindful. Immediate areas to provide valuable input is helping modelers navigate the modal aspects involved in various theory and models. How much can be identifying as pre-scripted categories from mathematics and how much will be observing systems with categorical aspects? This is a subtle difference, but from construct validity the directional ordering matters in these systems.

This would inevitably be an activity allowing system engineers the ability to document domain languages and theory for their linguistic and ordinal aspects. This would allow initially the ability to capture domains with minimal injection yet still providing a library and composition methods for these model domains. This is already a common activity for systems engineers, and the additional aspect will be maintaining not only 'bodies of knowledge' but the 'repertoire' of categorical transformations. Hopefully this could be a defined 'library' for socio-technical systems that provide domain model theory by indexing ordinal number, language constraint, and construct. How might this be accomplished?

Another point of usage from systems engineering would be to expand on the activity of tradespace construction. Involving ordinal constructs then leads to the question on how does one choice and trade over these aspects? This 'ordinal tradespace' would be a new concept and difficult to define. How does one do this a structured manner? As it is an incompleteness

measure, is there even a semi-numerical way this can be represented or accomplished? There is a certain paradox in discussing how to structure in a space assuming incomplete structures. As other areas have identified impossibility, incompleteness, and paradoxical aspects, the optimistic view is that this has challenged their disciplines to expand and provide strong explanations, methods, and theory respectively. Socio-technical systems are powerful notions given their construction, and one must not expect simple explanations but rather the objective is finding simple compressions across this domain.

7.3 FUTURE RESEARCH

Through the course of developing the approach documented in this section, a number of future research topics were identified that would allow for further refinement and improvement of enterprise modeling for the detection of unintended consequences. These research topics resulted from the major challenges encountered and described earlier in this report. In particular, for a truly robust and practical modeling approach one needs to have an inventory of potential models or theories that are relatively easy to navigate, select, and compose. The problem is that theories and models were never developed or organized for this purpose. Consequently, the following research topics were identified to facilitate this. It should be noted that it is expected that addressing these topics will be a long-term effort involving many researchers from many different disciplines.

1. Develop a theory for partitioning models for reuse

Most models are developed for a specific purpose. Consequently, no effort is made to minimize the possibility of transition linkages with other potentially related models. Is there a way, at least within a particular disciplinary area, to partition conceptual models in such a way to minimize transition linkages across developed models? If this could be done, model reuse and composition could be greatly facilitated.

2. Develop an organizational scheme for "refactored" models and theories

Assuming that one could refactor models and theories as described in topic 1, how should they be organized? Some models and theories will be complements, and others will be substitutes. Furthermore, different theories and models will exist at different layers of abstraction. Are there systematic ways to make the relationships among the refactored models and theories explicit and organized to facilitate search and composition?

3. Develop pasting rules for imperfect combinations of models

As discussed previously, it is unlikely that even related models can be refactored such that all potential transition linkages are eliminated. When these occur, we will find ourselves in either case 2 or case 3. Currently "handshake algorithms" or pasting functions are largely developed on an ad hoc basis. Are there any ground rules or heuristics that could accelerate the

development of these when necessary? If an experiment is required every time one wants to develop a new handshake, the utility of these models for practical policy analysis will diminish rapidly.

4. Develop a system for exploring variations on models

As noted previously, if one really were to build an inventory of composable models, it is unlikely that one would be able to evaluate every possible permutation for many policy questions. So, how should one select which variations to evaluate in such a large space? Could one develop distance metrics to guide the equivalent of a sensitivity analysis over model structure?

5. Develop a language for specifying model needs that logically determines the model composition and data integration scheme

When one transitions from the unrestricted conceptual model of the system to the more structured decomposable model structure (Figure 14c), how should one express that in order to facilitate model selection, composition, and experimentation? Can an existing formal language serve this purpose or must a new one be developed?

6. Integrate uncertainty quantification into the enterprise modeling approach

The ideal output of an enterprise policy analysis would be a probability distribution of outcomes (Figure 13d) rather than a set of scenario trajectories. In principle, this can be accomplished using Bayesian approaches, but there are likely to be computational issues. Consequently, uncertainty quantification techniques may need to be modified to accommodate the proposed system of varying model structure.

7. Develop an approach to integrate qualitative social science models into the model integration approach

Many social science theories are qualitative in nature, and it is not clear how they would be instantiated in a computational model. However, in abstract sense, they are still models, and should be mathematically representable. Is there a systematic way to integrate qualitative social science theories into a computational enterprise model? Category theory may play a role here.

8 REVISED ENTERPRISE MODELING METHODOLOGY

Based on the case studies and the analysis presented in this and previous reports, we propose several modifications to the original ten-step enterprise modeling methodology. Note that even in the original presentation of the methodology, it was not expected that it would be followed in an exact, sequential fashion. It was expected that in some cases not all of the steps would be necessary. In others, one may iterate through the steps several times. Consequently,

these revisions may be viewed as refinement of the same basic ideas that is based on a combination of experienced variations in enterprise model development as well as insights derived from the analysis of the literature and the theoretical analysis. The most important changes are a shift away from the development of a single, integrated computational instance to family of computational instances, and the introduction of three phases to manage the development, analysis, and communication of the family of computational instances.

The purpose of the phases is to both better manage the issues that arise from the integration of multi-scale ontologies as well as to systematically generate "counter-intuitive" results and "unintended consequences." To that end, the first phase involves laying out the key phenomena and developing a validated model of the "business as usual" case. We call this the core model, and it is the baseline against which we introduce model variations to identify unintended consequences. The second phase formally introduces variations as peripheral models that can be connected to or inserted into the core model. These are used to generate a set of possible scenarios that could be sources of unintended consequences. These potential scenarios are then evaluated for validity using a combination of data, experimentation, or subject matter expert (SME) review as appropriate. This allows a potentially large set of scenarios to be pared down to just those that are likely to be of concern to policymakers and stakeholders. The third phase focuses on communicating these key scenarios to policymakers and stakeholders. Interactive visualizations are developed to communicate the consequences of the key scenarios and the computational models are updated and integrated as necessary to support the interactive exploration of the scenarios. Finally, the findings are communicated via a group session where stakeholders and policymakers can interact with the simulation and visualizations.

Below are the detailed steps of the revised methodology. It should be noted that all ten of the original steps are present in some form. For each of the revised steps, linkages to the original ten steps are indicated by the step number in parentheses. To highlights the changes, new or modified steps are described using italicized text. As with the previous version of the methodology, it is not expected at all applications will involve an exact implementation of the steps. Rather they serve as general guidance. Furthermore, we have included recommended participants for each of the steps. These participants include:

- *Policymakers* are those in leadership positions that make final decisions regarding the selection of policy options and are held accountable for the resulting outcomes. These participants are often not concerned with the low-level details of the model but want to trust it.

- *Decision makers* are those in managerial positions below the policymakers. These mangers may be more detail oriented that the policymakers and want to verify the details of the model. Enterprise modeling efforts for small organizations may not include these participants.

- *Subject Matter Experts (SMEs)* are those with detailed knowledge and experience in specific aspects of the enterprise. Given that the enterprise modeling methodology

deliberately attempts to capture the enterprise from multiple perspectives, it is likely that the effort will involve subject matter experts from a diversity of backgrounds. These SMEs are often selected by the policymakers and/or decision makers. However, it is also important for the modelers to identify and engage SMEs on their own, when appropriate, to provide perspectives that the policymakers may not have considered.

- *Modelers* are those that are employing this enterprise modeling methodology. They coordinate participant interactions, collect data and information, set up the experimental design, develop the models, and perform the analysis.

- *Stakeholders* are those that may not have the authority to make policy but will be affected by consequences of any policy choices. Their buy-in is often required to make a policy effective.

1. Phase 1 – Identify, Model, and Validate the Core Relationships

1.1. Decide on the Central Questions of Interest (1)

The history of modeling and simulation is littered with failures of attempts to develop models without clear intentions in mind. Models provide means to answer questions. Efforts to model socio-technical systems are often motivated by decision makers' questions about the feasibility and efficacy of decisions on policy, strategy, operations, etc. The first step is to discuss the questions of interest with the decision maker(s), define what they need to know to feel that the questions are answered, and agree on key variables of interest.

Recommended participants: Stakeholders, Policymakers, Decision makers, SMEs, Modelers

1.2. Define Key Phenomena Underlying These Questions (2)

The next step involves defining the key phenomena that underlie the variables associated with the questions of interest. Phenomena can range from physical, behavioral, or organizational, to economic, social or political. *Particularly important are the relationships that link variables under the policymaker's control to outcomes of interest.* Broad classes of phenomena across these domains include continuous and discrete flows, manual and automatic control, resource allocation, and individual and collective choice. Mature domains often have developed standard descriptions of relevant phenomena.

Recommended participants: Stakeholders, Policymakers, Decision makers, SMEs, Modelers

1.3. Develop One or More Visualizations of Relationships among Phenomena (3)

Phenomena can often be described in terms of inputs, processes, and outputs. Often the inputs of one phenomenon are the outputs of other phenomena. Common variables among phenomena provide a basis for visualization of the set of key phenomena. Common visualizations methods include block diagrams, IDEF, influence diagrams, and systemigrams.

Recommended participants: SMEs, Modelers

1.4.   Determine Key Tradeoffs That Appear to Warrant Deeper Exploration (4)

The visualizations resulting from Step 1.3 often provide the basis for in-depth discussions and debates among members of the modeling team as well as the sponsors of the effort, which hopefully includes the decision makers who intend to use the results of the modeling effort to inform their decisions.   Lines of reasoning, perhaps only qualitative, are often verbalized that provides the means for immediate resolution of some issues, as well as dismissal of some issues that no longer seem to matter. New issues may, of course, also arise.

Recommended participants: Stakeholders, Policymakers, Decision makers, SMEs, Modelers

1.5.   Organize Phenomena into Core and Peripheral Groups (5)

Based on the key tradeoffs determined in step 1.4, we identify the control and response variables related to those tradeoffs and identify the relevant paths between them using the visualizations developed in step 1.3. These paths are candidates for establishing the core model. At a minimum, the core model must include at least one path from control to response, but multiple may be included. Presumably, the core will include what are perceived to be the most "important" factors. In essence, this would be the "first order" representation of the system. The phenomena that were omitted from the core are candidates to become peripheral models. Note that sometimes a peripheral model will be an alternative formulation of phenomena included in the core. This is of particular concern for behavioral and social factors where there may be alternative theories derived from different "schools."

Recommended participants: SMEs, Modelers

1.6.   Assess Types of Linkages among Phenomena (6)

Section 6 highlighted the different types of potential relationships that can occur among phenomena and associated approaches for capturing these computationally when dealing with multiple ontologies. Consequently, before designing any computational models, it is necessary to identify any transition linkages that may inhibit implementation.

Recommended participants: SMEs, Modelers

1.7.   Refactor to Create an Internally Consistent Core Model (7)

To provide a stable baseline for policy analysis, the core model must be internally consistent and generate accurate projections of the consequences of policy options to a first order. Consequently, the phenomena in the core model may need to be refactored using a combination of approaches described in Sections 6 and 7 to support the implementation of a computational model. The goal is to eliminate or account for any latent transition linkages

among phenomena captured using different ontologies. This may involve both substituting representations and introducing "handshakes."

Recommended participants: Modelers

1.8. Architect Simulation Based on Linkages among the Core and Peripheral Groups (5,6,7)

The implementation decisions of the core model may impact how the peripheral models will be connected or inserted. Consequently, it is advisable to develop a simulation architecture to guide to the development of both the core model and any peripheral models. Otherwise, a particular computational implementation of the core may preclude the introduction of a particular peripheral model. Completion of this step may require iteration with step 1.7.

Recommended participants: Modelers

1.9. Identify Data Sets to Parameterize the Core Model (8)

The set of representations chosen and refined *in step 1.8* will have parameters such as transition probabilities, time constants, and decay rates that have to be estimated using data from the domain(s) in which the questions of interest are to be addressed. Data sources need to be identified and conditions under which these data were collected determined. Estimation methods need to be chosen, and in some cases developed, to provide unbiased estimates of model parameters. *The emphasis in this phase is on parameterizing and calibrating the core model to ensure that it is consistent with available data and SME expectations.*

Recommended participants: SMEs, Modelers

1.10. Program and Verify the core model (9)

To the extent possible, this step is best accomplished with commercially available software tools. The prototyping and debugging capabilities of such tools are often well worth the price. A variant of this proposal is to use commercial tools to prototype and refine the overall model. Once the design of the model is fixed, one can then develop custom software for production runs. The versions in the commercial tools can then be used to verify the custom code. *In this step we are less concerned with interface development and more concerned with generating accurate results and supporting subsequent analysis using the peripheral models.*

Recommended participants: Modelers

1.11. Validate Core Model Predictions at Least against Baseline Data (10)

The core model is validated by using it to predict current performance with the "as is" policies, strategies, etc. Empirical data is ideal, but in low data environments, SME review

may suffice. Here the objective is not to generate "what if" scenarios, but rather to demonstrate that the model is able to capture what is already known and understood.

Recommended participants: SMEs, Modelers, Decision makers

2. **Phase 2 – Introduce and Model Peripheral Relationships to Generate Scenarios**

   2.1. *Organize Peripheral Groups Into an Experimental Design*

   While analysts and modelers have experimented using alternative model structure in the past, the goal here is to conduct the analysis in a systematic way. Consequently, a plan should be developed to introduce peripheral models to the core and capture at minimum the qualitative changes in the in the predicated outcomes. Confounding of results should be kept to a minimum. While the approach described in Section 7 is minimally sufficient, a model repository as described in the RT-110 report (Pennock et al 2015) and progress against the described future research topics could greatly facilitate this step.

   Recommended participants: SMEs, Modelers

   2.2. *Identify Data Sets to Parameterize Peripheral Models as Appropriate (8)*

   Similar to Step 1.9, the peripheral models will require some parametrization. Depending on the experimental design, additional data may or may not be required. For certain "what if" experiments, it may be desirable to explore circumstances which have never been experienced. Other experiments may involve an alternative formulation of an aspect of the core. In those cases, it may be necessary to parametrize the using the same data as the core.

   Recommended participants: SMEs, Modelers

   2.3. *Program and Verify the Peripheral-Core Variations to Support Experimental Design (9)*

   Often this step will involve the same tools used in step 1.10. However this is not strictly required. For example, in some circumstances, a peripheral model may be implemented in a specialized tool and then key outputs are communicated to the core. This will be heavily dependent on the nature of the peripheral models and the types of linkage relationships between the peripheral model and the core. As with step 1.10, we are less concerned with interface development and more concerned with generating a wide range of potentially useful scenarios.

   Recommended participants: Modelers

   2.4. *Generate Scenarios According to Experimental Design*

   This step executes the production runs to satisfy the experimental design from step 1.2. Depending on the design, the number of scenarios may be substantial. Results should not be filtered or validated at this point. Due to uncertainties in model structure and parameters, it

may only be possible to identify qualitative differences from the predictions of the core model. At this point, we are less concerned with predictive accuracy and more concerned with not missing a potential "unintended consequence."

Recommended participants: Modelers

2.5. Validate and Trim Scenario Set using Data, Experiments, and SME Review

It is likely that the experimental design will generate a very large number of potential scenarios. However, not all may be relevant. Some may not be significantly different from the predictions of core models. Others may be infeasible due to factors excluded from the model. SME review could be useful to weed these out. Finally, when possible, scenarios could be tested using experiments or by collecting additional data. It is important to note, though, that given the objective is to detect unintended consequences, a high threshold should be set to reject a scenario. When in doubt, it may be better to retain a scenario that is significantly different from the core projections. Even if the projection is not entirely accurate, its existence may be informative to policymakers and stakeholders.

Recommended participants: SMEs, Modelers, Decision makers

3. Phase 3 – Communicate with Stakeholders via Interactive Interface and Visualizations

3.1. Identify Scenarios That Appear to Warrant Communication to Stakeholders (4)

Based on the questions of interest, key tradeoffs, and the outputs of Step 2.5, identify the scenarios that are most relevant to policy stakeholders. It is unlikely that modelers will have time to go through all possible scenarios with stakeholders, at least in the first session (and this may actually be counterproductive). Also when developing interactive interfaces and visualizations in the subsequent steps, there is often a tradeoff between the number of possible variations that the interfaces accommodate and the interpretability of those interfaces by the stakeholders. Instead, highlight those that are both relevant to the questions of interest and reveal possibilities that may be unexpected for the stakeholders. Of course, follow up discussions may lead to modifications of this set.

Recommended participants: SMEs, Modelers, Decision makers

3.2. Develop One or More Visualizations that Explain Relationships among Policy Options and Potential Scenarios (3)

In order to communicate the findings to stakeholders, develop visualizations that clearly explain the linkage between the decision variables and outcomes interest. Also ensure that these visualizations can properly discriminate between the various scenarios that are being presented. The emphasis is on communicating the key scenarios as opposed to developing a visualization that can accommodate all possible scenarios.

Recommended participants: SMEs, Modelers

3.3. Selectively Modify or Integrate Computational Instantiations to Generate Visualizations (9)

In order to support the exploration of scenarios using the interactive visualization, it may be necessary to modify the production level simulations. In some cases this may be as simple as hiding some input controls to highlight the most relevant. In cases where the simulation is computationally intensive, it may be necessary to summarize a large number of runs using response surfaces, fit statistical models, etc.

Recommended participants: Modelers

3.4. Develop an Interactive Interface to allow for "on-the-fly" exploration of scenarios

This step involves instantiating interactive visualizations with graphs, charts, sliders, radio buttons, etc. Commercial and open source tools may be useful for making attractive and easy to use interfaces. Interfaces that are scalable to large displays and/or touchscreens are ideal to facilitate group interaction.

Recommended participants: Modelers

3.5. Communicate Findings to Stakeholders via Interactive Visualizations

In order to communicate the results of the analysis, it is useful to let policymakers and stakeholders directly interact with the visualizations and/or modified simulation tools. Ideally, this can be done in a group setting where interactions with the visualization trigger discussions and exploration of scenarios. This step may result in the identification of "what if" scenarios that cannot be accommodated with the current computational instantiation. This may require returning to earlier steps to address these new scenarios.

Recommended participants: Stakeholders, Policymakers, Decision makers, SMEs, Modelers

9 CONCLUSIONS

The primary objectives of RT-161 were to evaluate the core-peripheral concept against a new case study, develop an approach to deal with multi-scale ontologies, and develop an approach to systematically identify unintended policy consequences. Based on the satisfaction of these objectives, the enterprise modeling approach was to be updated. The net result of completing this work was a substantial revision of the enterprise modeling methodology. More specifically, the core-peripheral approach was found to be useful, and as a result, it was explicitly incorporated into the methodology. Furthermore, the detailed literature review and a theoretical investigation led to an approach to partition an enterprise system across multi-scale ontologies to generate the core and peripheral models. The peripheral models are systematically introduced via an experimental design to identify unintended consequences in a justifiable and explainable way. Ultimately, this lead to the reorganization of the enterprise

modeling methodology into three major phases. Each phase contains a number of detailed steps that should provide additional guidance to enterprise analysts above and beyond what was provided by previous versions.

Beyond the updates to the methodology, completion of RT-161 led to several research conclusions:

- The core-peripheral approach to enterprise analysis is promising, but will require additional test cases to confirm its efficacy

- The original ten-steps of the enterprise modeling methodology required additional refinement and expansion to both support the proper validation of the model and systematic detection of unintended policy consequences. This led to a reorganization of the ten steps into three phases. The first phase focuses on understanding the problem and developing and validating the core. The second phase systematically introduces the peripheral models to identify unintended policy consequences, and the third phase communicates key findings to enterprise stakeholders.

- The problem of dealing with multi-scale ontologies for discovery does not appear to have a general solution in either the physical sciences or the social sciences. In the physical sciences, multi-scale models tend to devolve to interpolation as opposed to discovery. In the social sciences, we have the opposite problem as the number of different possible explanations of a phenomena tend to proliferate resulting in sometimes inconsistent predictions or predictions are that are accurate for groups but not individuals. Consequently, there is a continual struggle for "construct validity."

- If one is going to successfully predict unintended policy outcomes for enterprise systems, properly organizing and leveraging this myriad of social science representations is key. Consequently, there are important research questions as to how to go about this in a mathematically rigorous way.

- Model composition problems experienced in multi-scale models may be the result of latent transition linkages among the different models. Identifying and managing these linkages through proper partitioning schemes may be the key to facilitating this type of analysis.

- One possible approach for describing, organizing, and relating diverse system models is through the application of a branch of mathematics called Category Theory. At a minimum, it may provide a language to rigorously describe the problem, but much additional research is required.

These conclusions led us to describe several potential avenues for further improvements in the enterprise modeling methodology. Among these avenues are a rigorous approach to partitioning and refactoring models for reuse, adapting the concept of a "nomological network" from the social sciences to the organization of candidate models for use in an enterprise analysis, and directly integrating uncertainty quantification approaches into the enterprise

modeling methodology. However, since these activities were outside of the scope of this research task, they must be relegated to future work.

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